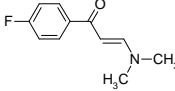


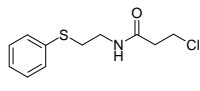


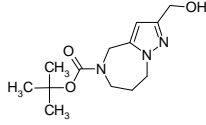
BIONET compounds –
A Key step ahead of the rest

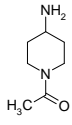
3 April 20#0
Fragments Collection Update

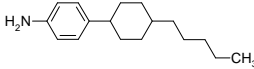
 **Key Organics**
The right side of the Equation

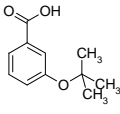
10C-067	C ₁₁ H ₁₂ FNO	193.2228	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>1.8698</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	4.0000	H-bond acceptors	1.0000	H-bond donors	0.0000	LogP	1.8698
Halogen atoms	1.0000												
rotatable bonds	4.0000												
H-bond acceptors	1.0000												
H-bond donors	0.0000												
LogP	1.8698												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(dimethylamino)-1-(4-fluorophenyl)-2-propen-1-one													

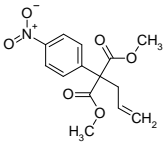
10K-539S	C ₁₁ H ₁₄ ClNOS	243.7573	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>6.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.9456</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	6.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	1.9456
Halogen atoms	1.0000												
rotatable bonds	6.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	1.9456												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-chloro-N-[2-(phenylsulfanyl)ethyl]propanamide													

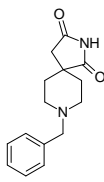
10X-0603	C ₁₃ H ₂₁ N ₃ O ₃	267.3306	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.7722</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	0.7722
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	0.7722												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
tert-butyl 2-(hydroxymethyl)-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxylate													

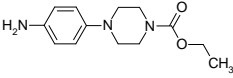
11X-0603	C ₇ H ₁₄ N ₂ O	142.2024	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>-1.3333</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	0.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	-1.3333
Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	-1.3333												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(4-aminopiperidino)-1-ethanone													

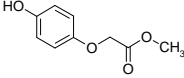
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	0.0000												
H-bond donors	1.0000												
LogP	5.0580												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(4-pentylcyclohexyl)aniline													

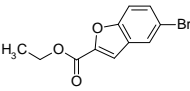
12P-016	C ₁₁ H ₁₄ O ₃	194.2324	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.3261</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.3261
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.3261												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(tert-butoxy)benzenecarboxylic acid													

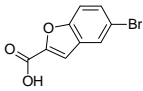
12T-0017	C ₁₄ H ₁₅ NO ₆	293.2788	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>7.0000</td></tr> <tr><td>H-bond acceptors</td><td>6.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.7307</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	7.0000	H-bond acceptors	6.0000	H-bond donors	0.0000	LogP	2.7307
Halogen atoms	0.0000												
rotatable bonds	7.0000												
H-bond acceptors	6.0000												
H-bond donors	0.0000												
LogP	2.7307												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
dimethyl 2-allyl-2-(4-nitrophenyl)malonate													

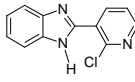
1R-1514	C ₁₅ H ₁₈ N ₂ O ₂	258.3229	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.1152</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.1152
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.1152												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
8-benzyl-2,8-diazaspiro[4.5]decane-1,3-dione													


1X-0601	$C_{13}H_{19}N_3O_2$	249.3153		Halogen atoms 0.0000 rotatable bonds 3.0000 H-bond acceptors 2.0000 H-bond donors 1.0000 LogP 1.1279
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
ethyl 4-(4-aminophenyl)tetrahydro-1(2H)-pyrazinecarboxylate				

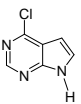
2R-0144	$C_9H_{10}O_4$	182.1777		Halogen atoms 0.0000 rotatable bonds 4.0000 H-bond acceptors 4.0000 H-bond donors 1.0000 LogP 1.0830
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
methyl 2-(4-hydroxyphenoxy)acetate				

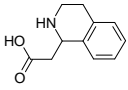
2Y-0815	$C_{11}H_9BrO_3$	269.0966		Halogen atoms 1.0000 rotatable bonds 3.0000 H-bond acceptors 3.0000 H-bond donors 0.0000 LogP 2.6258
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
ethyl 5-bromo-1-benzofuran-2-carboxylate				

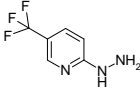
2Y-0823	$C_9H_5BrO_3$	241.0424		Halogen atoms 1.0000 rotatable bonds 1.0000 H-bond acceptors 3.0000 H-bond donors 1.0000 LogP 2.2516
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
5-bromo-1-benzofuran-2-carboxylic acid				

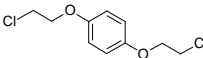
3J-543S	$C_{12}H_8ClN_3$	229.6707		Halogen atoms 1.0000 rotatable bonds 1.0000 H-bond acceptors 2.0000 H-bond donors 1.0000 LogP 2.6905
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
2-(2-chloro-3-pyridinyl)-1H-1,3-benzimidazole				

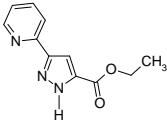
3K-345S	$C_3H_6N_4S$	130.1721		Halogen atoms 0.0000 rotatable bonds 1.0000 H-bond acceptors 3.0000 H-bond donors 1.0000 LogP 0.8557
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
5-(1-methylhydrazino)-1,2,3-thiadiazole				

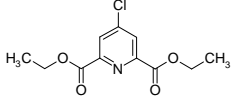
3Z-0603	$C_6H_4ClN_3$	153.5719		Halogen atoms 1.0000 rotatable bonds 0.0000 H-bond acceptors 2.0000 H-bond donors 1.0000 LogP 1.5106
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
4-chloro-7H-pyrrolo[2,3-d]pyrimidine				

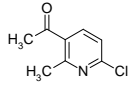
4H-048	$C_{11}H_{13}NO_2$	191.2318		Halogen atoms 0.0000 rotatable bonds 2.0000 H-bond acceptors 3.0000 H-bond donors 2.0000 LogP 1.3475
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
2-(1,2,3,4-tetrahydro-1-isoquinolinyl)acetic acid				

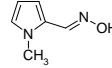
4R-0680	$C_6H_6F_3N_3$	177.1300											
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	2.0956												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-hydrazino-5-(trifluoromethyl)pyridine													

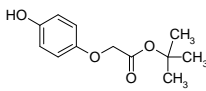
4Y-0018	$C_{10}H_{12}Cl_2O_2$	235.1119											
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Halogen atoms	2.0000												
rotatable bonds	6.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	2.9484												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1,4-bis(2-chloroethoxy)benzene													


5Z-0611	$C_{11}H_{11}N_3O_2$	217.2292											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.3815												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 3-(2-pyridinyl)-1H-pyrazole-5-carboxylate													

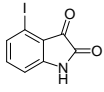
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Halogen atoms	1.0000												
rotatable bonds	6.0000												
H-bond acceptors	5.0000												
H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
diethyl 4-chloro-2,6-pyridinedicarboxylate													

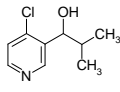
6R-0618	C_8H_8ClNO	169.6121											
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Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	1.5813												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(6-chloro-2-methyl-3-pyridinyl)-1-ethanone													

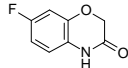
7P-087	$C_6H_8N_2O$	124.1435											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.3971												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-methyl-1H-pyrrole-2-carbaldehyde oxime													

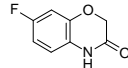
7R-0603	$C_{12}H_{16}O_4$	224.2589											
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.9168												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
tert-butyl 2-(4-hydroxyphenoxy)acetate													

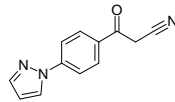
9N-013	$C_5H_4N_2O_2$	124.0998											
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	0.1881												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-pyrimidinecarboxylic acid													

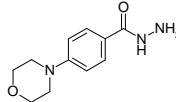
9P-718	C ₈ H ₄ INO ₂	273.0310											
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.3813												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-iodo-1H-indole-2,3-dione													

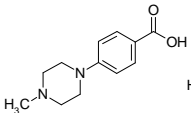
AB-5006	C ₉ H ₁₂ ClNO	185.6551											
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.4668												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(4-chloro-3-pyridinyl)-2-methyl-1-propanol													

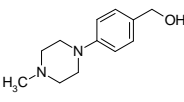
AD-0189	C ₈ H ₆ FNO ₂	167.1409											
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	0.4920												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
7-fluoro-2H-1,4-benzoxazin-3(4H)-one													

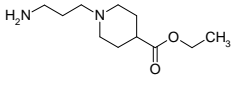
AD-0189	C ₈ H ₆ FNO ₂	167.1409											
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	0.4920												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
7-fluoro-2H-1,4-benzoxazin-3(4H)-one													

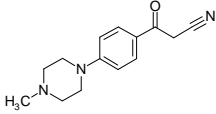
AD-0212	C ₁₂ H ₉ N ₃ O	211.2250											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	1.8690												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-oxo-3-[4-(1H-pyrazol-1-yl)phenyl]propanenitrile													

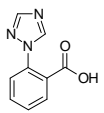
AD-0295	C ₁₁ H ₁₅ N ₃ O ₂	221.2611											
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rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	0.3168												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-morpholinobenzenecarbohydrazide													

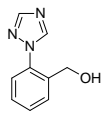
AD-0334	C ₁₂ H ₁₇ ClN ₂ O ₂	256.7345											
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.6468												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(4-methylpiperazin-1-yl)benzoic acid hydrochloride													

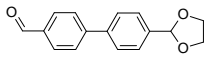
AD-0335	C ₁₂ H ₁₈ N ₂ O	206.2901											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.1046												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
[4-(4-methylpiperazino)phenyl]methanol													

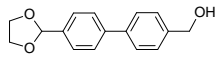
AD-0363	$C_{11}H_{22}N_2O_2$	214.3102
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		rotatable bonds
		6.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	-0.1557	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
ethyl 1-(3-aminopropyl)-4-piperidinecarboxylate		

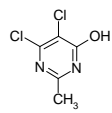
AD-0365	$C_{14}H_{17}N_3O$	243.3111
		Halogen atoms
		0.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
0.0000		
LogP	0.9744	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
3-[4-(4-methylpiperazino)phenyl]-3-oxopropanenitrile		

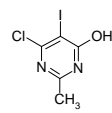
AD-0730	$C_9H_7N_3O_2$	189.1750
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		rotatable bonds
		2.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	1.5998	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-(1H-1,2,4-triazol-1-yl)benzenecarboxylic acid		

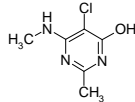
AD-0738	$C_9H_9N_3O$	175.1916
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		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	1.3661	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
[2-(1H-1,2,4-triazol-1-yl)phenyl]methanol		

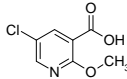
AD-0750	$C_{16}H_{14}O_3$	254.2882
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		0.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
0.0000		
LogP	3.1445	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
4'-(1,3-dioxolan-2-yl)[1,1'-biphenyl]-4-carbaldehyde		

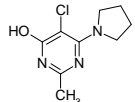
AD-0761	$C_{16}H_{16}O_3$	256.3041
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		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	2.9337	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
[4'-(1,3-dioxolan-2-yl)[1,1'-biphenyl]-4-yl]methanol		

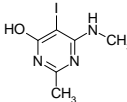
AD-0773	$C_5H_4Cl_2N_2O$	179.0064
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		2.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	2.0600	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
5,6-dichloro-2-methyl-4-pyrimidinol		

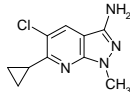
AD-0790	$C_5H_4ClIN_2O$	270.4578
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		rotatable bonds
		0.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	2.7994	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
6-chloro-5-iodo-2-methyl-4-pyrimidinol		

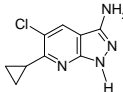
AD-0791	C ₆ H ₈ ClN ₃ O	173.6032	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
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		H-bond donors	2.0000
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-chloro-2-methyl-6-(methylamino)-4-pyrimidinol			

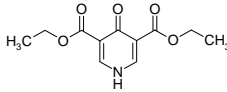
AD-5000	C ₇ H ₆ ClNO ₃	187.5838	
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		rotatable bonds	2.0000
		H-bond acceptors	4.0000
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		LogP	1.8619
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-chloro-2-methoxynicotinic acid			

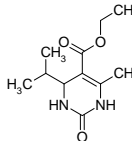
AD-5001	C ₉ H ₁₂ ClN ₃ O	213.6685	
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		H-bond donors	1.0000
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-chloro-2-methyl-6-(1-pyrrolidinyl)-4-pyrimidinol			

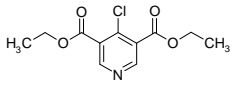
AD-5002	C ₆ H ₈ IN ₃ O	265.0546	
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		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-iodo-2-methyl-6-(methylamino)-4-pyrimidinol			

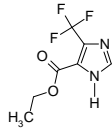
AD-5012	C ₁₀ H ₁₁ ClN ₄	222.6790	
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		H-bond donors	1.0000
		LogP	2.2833
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-chloro-6-cyclopropyl-1-methyl-1H-pyrazolo[3,4-b]pyridin-3-amine			

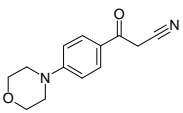
AD-5013	C ₉ H ₉ ClN ₄	208.6519	
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		LogP	2.0368
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-chloro-6-cyclopropyl-1H-pyrazolo[3,4-b]pyridin-3-ylamine			

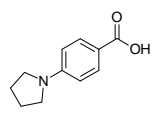
BD-0078	C ₁₁ H ₁₃ NO ₅	239.2300	
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		H-bond donors	1.0000
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
diethyl 4-oxo-1,4-dihydro-3,5-pyridinedicarboxylate			

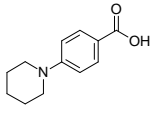
BD-0109	C ₁₁ H ₁₈ N ₂ O ₃	226.2777	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
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		H-bond donors	2.0000
		LogP	0.0018
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 4-isopropyl-6-methyl-2-oxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

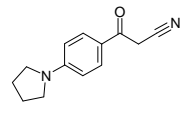
BD-0110	$C_{11}H_{12}ClNO_4$	257.6756											
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Halogen atoms	1.0000												
rotatable bonds	6.0000												
H-bond acceptors	5.0000												
H-bond donors	0.0000												
LogP	1.8628												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
diethyl 4-chloro-3,5-pyridinedicarboxylate													

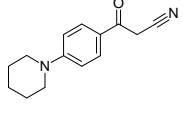
BD-0119	$C_7H_7F_3N_2O_2$	208.1412											
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Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.8712												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 4-(trifluoromethyl)-1H-imidazole-5-carboxylate													

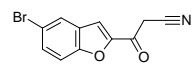
BD-0200	$C_{13}H_{14}N_2O_2$	230.2687											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>0.8305</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	0.8305	
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	0.8305												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(4-morpholinophenyl)-3-oxopropanenitrile													

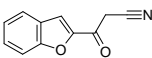
BD-0212	$C_{11}H_{13}NO_2$	191.2318											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.8626												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(1-pyrrolidinyl)benzenecarboxylic acid													

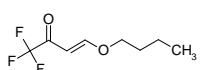
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.2589												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-piperidinobenzenecarboxylic acid													

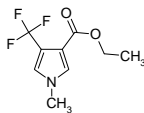
BD-0221	$C_{13}H_{14}N_2O$	214.2693											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	1.4987												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-oxo-3-[4-(1-pyrrolidinyl)phenyl]propanenitrile													

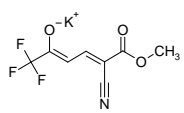
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-oxo-3-(4-piperidinophenyl)propanenitrile													

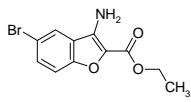
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	1.8877												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(5-bromo-1-benzofuran-2-yl)-3-oxopropanenitrile													

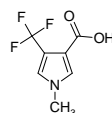
BD-0229	$C_{11}H_7NO_2$	185.1839	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>1.0959</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	1.0959
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	1.0959												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(1-benzofuran-2-yl)-3-oxopropanenitrile													

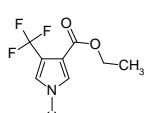
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Halogen atoms	3.0000												
rotatable bonds	6.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	2.0914												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-butoxy-1,1,1-trifluoro-3-buten-2-one													

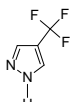
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Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	2.2553												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 1-methyl-4-(trifluoromethyl)-1H-pyrrole-3-carboxylate													

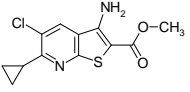
BD-0268	$C_8H_5F_3KNO_3$	259.2311	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td></td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td></td></tr> </table>	Halogen atoms	3.0000	rotatable bonds		H-bond acceptors	4.0000	H-bond donors	0.0000	LogP	
Halogen atoms	3.0000												
rotatable bonds													
H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP													
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
potassium 5-cyano-1,1,1-trifluoro-6-methoxy-2,4-hexadien-2-olate													

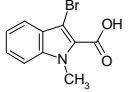
BD-0274	$C_{11}H_{10}BrNO_3$	284.1113	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.8426</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.8426
Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.8426												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 3-amino-5-bromo-1-benzofuran-2-carboxylate													

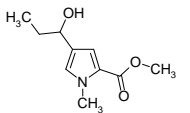
BD-0278	$C_7H_6F_3NO_2$	193.1266	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.8811</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	1.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	1.8811
Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.8811												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-methyl-4-(trifluoromethyl)-1H-pyrrole-3-carboxylic acid													

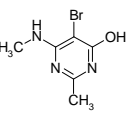
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Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 4-(trifluoromethyl)-1H-pyrrole-3-carboxylate													

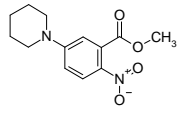
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Halogen atoms	3.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	1.2568												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(trifluoromethyl)-1H-pyrazole													

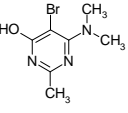
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		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.0326
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 3-amino-5-chloro-6-cyclopropylthieno[2,3-b]pyridine-2-carboxylate			

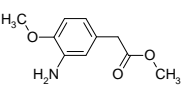
BD-0701	C ₁₀ H ₈ BrNO ₂	254.0848	
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		H-bond donors	1.0000
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-bromo-1-methyl-1H-indole-2-carboxylic acid			

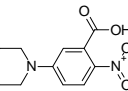
BD-0702	C ₁₀ H ₁₅ NO ₃	197.2360	
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		rotatable bonds	4.0000
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		H-bond donors	1.0000
		LogP	1.1406
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 4-(1-hydroxypropyl)-1-methyl-1H-pyrrole-2-carboxylate			

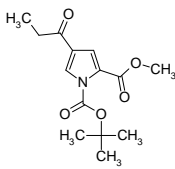
BD-0706	C ₆ H ₈ BrN ₃ O	218.0542	
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		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	1.5743
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-bromo-2-methyl-6-(methylamino)-4-pyrimidinol			

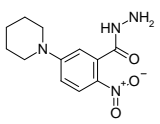
BD-0708	C ₁₃ H ₁₆ N ₂ O ₄	264.2835	
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		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	2.2442
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-nitro-5-piperidinobenzenecarboxylate			

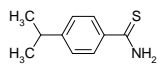
BD-0711	C ₇ H ₁₀ BrN ₃ O	232.0813	
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		H-bond donors	1.0000
		LogP	1.9357
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5-bromo-6-(dimethylamino)-2-methyl-4-pyrimidinol			

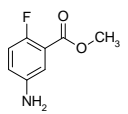
BD-0715	C ₁₀ H ₁₃ NO ₃	195.2200	
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-(3-amino-4-methoxyphenyl)acetate			

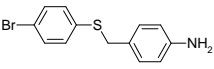
BD-0716	C ₁₂ H ₁₄ N ₂ O ₄	250.2564	
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		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details
2-nitro-5-piperidinobenzenecarboxylic acid			

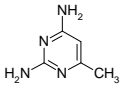
BD-0717	C ₁₄ H ₁₉ NO ₅	281.3112
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	rotatable bonds	6.0000
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	H-bond donors	0.0000
	LogP	1.9416
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
1-(tert-butyl) 2-methyl 4-propionyl-1H-pyrrole-1,2-dicarboxylate		

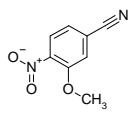
BD-0719	C ₁₂ H ₁₆ N ₄ O ₃	264.2863
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	rotatable bonds	2.0000
	H-bond acceptors	4.0000
	H-bond donors	2.0000
	LogP	1.3349
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
2-nitro-5-piperidinobenzenecarbohydrazide		

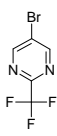
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	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
4-isopropylbenzenecarbothioamide		

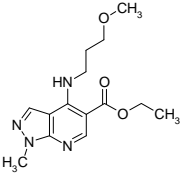
BD-0725	C ₈ H ₈ FNO ₂	169.1569
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	rotatable bonds	2.0000
	H-bond acceptors	2.0000
	H-bond donors	1.0000
	LogP	1.1330
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
methyl 5-amino-2-fluorobenzenecarboxylate		

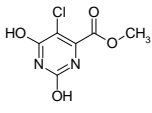
BD-0727	C ₁₃ H ₁₂ BrNS	294.2153
	Halogen atoms	1.0000
	rotatable bonds	3.0000
	H-bond acceptors	0.0000
	H-bond donors	1.0000
	LogP	3.9224
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
4-(((4-bromophenyl)sulfanyl)methyl)aniline		

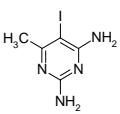
BD-0732	C ₅ H ₈ N ₄	124.1463
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	rotatable bonds	0.0000
	H-bond acceptors	2.0000
	H-bond donors	2.0000
	LogP	0.3753
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
6-methyl-2,4-pyrimidinediamine		

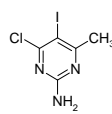
BD-0733	C ₈ H ₆ N ₂ O ₃	178.1486
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	rotatable bonds	1.0000
	H-bond acceptors	4.0000
	H-bond donors	0.0000
	LogP	1.6125
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
3-methoxy-4-nitrobenzenecarbonitrile		

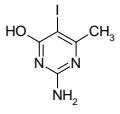
BD-0736	C ₅ H ₂ BrF ₃ N ₂	226.9843
	Halogen atoms	4.0000
	rotatable bonds	0.0000
	H-bond acceptors	2.0000
	H-bond donors	0.0000
	LogP	2.4277
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
5-bromo-2-(trifluoromethyl)pyrimidine		

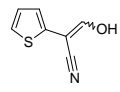
CB-0059	$C_{14}H_{20}N_4O_3$	292.3405
		Halogen atoms
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		rotatable bonds
		8.0000
		H-bond acceptors
		5.0000
H-bond donors		
1.0000		
LogP	0.2236	
LogS	contact Key Organics for details	TPSA
ethyl 4-[(3-methoxypropyl)amino]-1-methyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate		

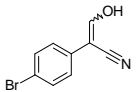
CD-0006	$C_6H_5ClN_2O_4$	204.5708
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		rotatable bonds
		2.0000
		H-bond acceptors
		6.0000
H-bond donors		
2.0000		
LogP	1.3707	
LogS	contact Key Organics for details	TPSA
methyl 5-chloro-2,6-dihydroxy-4-pyrimidinecarboxylate		

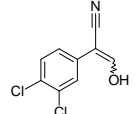
CD-0020	$C_5H_7IN_4$	250.0427
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		rotatable bonds
		0.0000
		H-bond acceptors
		2.0000
H-bond donors		
2.0000		
LogP	1.6327	
LogS	contact Key Organics for details	TPSA
5-iodo-6-methyl-2,4-pyrimidinediamine		

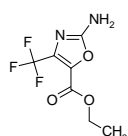
CD-0041	$C_5H_5ClIN_3$	269.4731
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		rotatable bonds
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		2.0000
H-bond donors		
1.0000		
LogP	2.6060	
LogS	contact Key Organics for details	TPSA
4-chloro-5-iodo-6-methyl-2-pyrimidinamine		


CD-0062	$C_5H_6IN_3O$	251.0275
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		rotatable bonds
		0.0000
		H-bond acceptors
		3.0000
H-bond donors		
2.0000		
LogP	2.1315	
LogS	contact Key Organics for details	TPSA
2-amino-5-iodo-6-methyl-4-pyrimidinol		

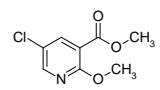
CD-0084	C_7H_5NOS	151.1880
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		2.0000
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H-bond donors		
1.0000		
LogP	1.0842	
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3-hydroxy-2-(2-thienyl)acrylonitrile		

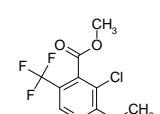
CD-0085	C_9H_6BrNO	224.0583
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		2.0000
		H-bond acceptors
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H-bond donors		
1.0000		
LogP	2.5843	
LogS	contact Key Organics for details	TPSA
2-(4-bromophenyl)-3-hydroxyacrylonitrile		

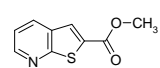
CD-0105	$C_9H_6Cl_2NO$	214.0523
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		rotatable bonds
		2.0000
		H-bond acceptors
		2.0000
H-bond donors		
1.0000		
LogP	2.8285	
LogS	contact Key Organics for details	TPSA
2-(3,4-dichlorophenyl)-3-hydroxyacrylonitrile		

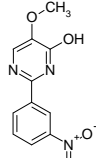
CD-0201	$C_7H_7F_3N_2O_3$	224.1406	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.1749</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	1.1749
Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.1749												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 2-amino-4-(trifluoromethyl)-1,3-oxazole-5-carboxylate													

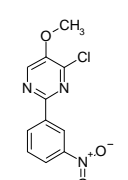
CD-0251	$C_5H_3F_3N_2O$	164.0877	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.7867</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.7867
Halogen atoms	3.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.7867												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-(trifluoromethyl)-4-pyrimidinol													

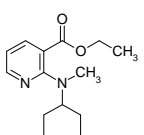
CD-0700	$C_8H_8ClNO_3$	201.6109	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>1.8936</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	0.0000	LogP	1.8936
Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 5-chloro-2-methoxynicotinate													

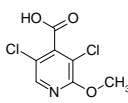
CD-0705	$C_9H_7ClF_3NO_3$	269.6092	<table border="1"> <tr><td>Halogen atoms</td><td>4.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.3115</td></tr> </table>	Halogen atoms	4.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	0.0000	LogP	2.3115
Halogen atoms	4.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP	2.3115												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 3-chloro-2-methoxy-5-(trifluoromethyl)isonicotinate													

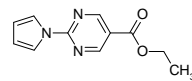
CD-0707	$C_9H_7NO_2S$	193.2256	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>1.2810</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	1.2810
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	1.2810												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl thieno[2,3-b]pyridine-2-carboxylate													

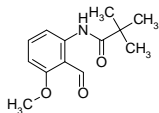
CD-0710	$C_{11}H_9N_3O_4$	247.2121	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>6.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.5526</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	6.0000	H-bond donors	1.0000	LogP	2.5526
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	6.0000												
H-bond donors	1.0000												
LogP	2.5526												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-methoxy-2-(3-nitrophenyl)-4-pyrimidinol													

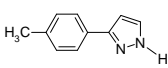
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	5.0000												
H-bond donors	0.0000												
LogP	3.0271												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-chloro-5-methoxy-2-(3-nitrophenyl)pyrimidine													

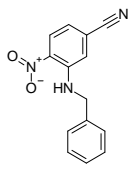
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.8830												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 2-(cyclohexyl(methyl)amino)nicotinate													

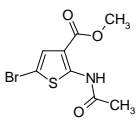
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Halogen atoms	2.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.9150												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3,5-dichloro-2-methoxyisonicotinic acid													

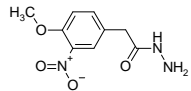
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 2-(1H-pyrrol-1-yl)-5-pyrimidinecarboxylate													

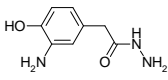
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.1740												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-(2-formyl-3-methoxyphenyl)-2,2-dimethylpropanamide													

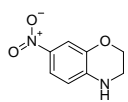
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(4-methylphenyl)-1H-pyrazole													

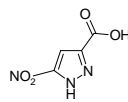
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	3.0724												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(benzylamino)-4-nitrobenzenecarbonitrile													

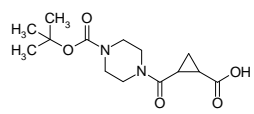
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Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.5292												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 2-(acetylamino)-5-bromo-3-thiophenecarboxylate													

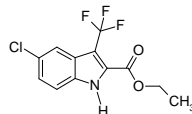
CD-0739	$C_9H_{11}N_3O_4$	225.2057											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	5.0000												
H-bond donors	2.0000												
LogP	0.5008												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(4-methoxy-3-nitrophenyl)acetohydrazide													

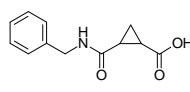
CD-0742	$C_8H_{11}N_3O_2$	181.1958											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	4.0000												
LogP	-0.2677												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(3-amino-4-hydroxyphenyl)acetohydrazide													

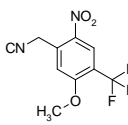
CD-0744	$C_8H_8N_2O_3$	180.1646											
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rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.0003												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
7-nitro-3,4-dihydro-2H-1,4-benzoxazine													

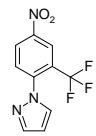
CD-0745	$C_4H_3N_3O_4$	157.0862											
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	5.0000												
H-bond donors	2.0000												
LogP	0.3678												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-nitro-1H-pyrazole-3-carboxylic acid													

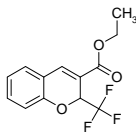
DD-0044	$C_{14}H_{22}N_2O_5$	298.3418											
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rotatable bonds	4.0000												
H-bond acceptors	5.0000												
H-bond donors	1.0000												
LogP	0.0405												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[(4-(tert-butoxycarbonyl)piperazinyl)carbonyl]cyclopropanecarboxylic acid													

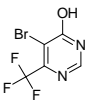
DD-0047	$C_{12}H_9ClF_3NO_2$	291.6592											
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rotatable bonds	3.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	3.0574												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 5-chloro-3-(trifluoromethyl)-1H-indole-2-carboxylate													

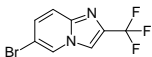
DD-0051	$C_{12}H_{13}NO_3$	219.2423											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	1.0068												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[(benzylamino)carbonyl]cyclopropanecarboxylic acid													

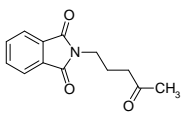
DD-0057	$C_{10}H_7F_3N_2O_3$	260.1741											
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Halogen atoms	3.0000												
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H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP	2.4278												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[5-methoxy-2-nitro-4-(trifluoromethyl)phenyl]acetonitrile													

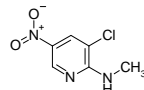
DD-0060	$C_{10}H_6F_3N_3O_2$	257.1734											
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	3.3709												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-[4-nitro-2-(trifluoromethyl)phenyl]-1H-pyrazole													

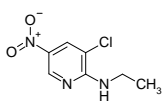
DD-0210	$C_{13}H_{11}F_3O_3$	272.2260											
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Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.8607												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 2-(trifluoromethyl)-2H-chromene-3-carboxylate													

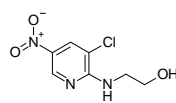
DD-0212	$C_5H_2BrF_3N_2O$	242.9837
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		rotatable bonds
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		H-bond acceptors
3.0000		
H-bond donors		
1.0000		
LogP	2.5785	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
5-bromo-6-(trifluoromethyl)-4-pyrimidinol		

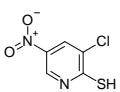
DD-0214	$C_8H_4BrF_3N_2$	265.0337
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		rotatable bonds
		0.0000
		H-bond acceptors
1.0000		
H-bond donors		
0.0000		
LogP	2.4900	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
6-bromo-2-(trifluoromethyl)imidazo[1,2-a]pyridine		

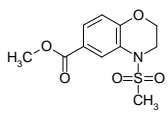
DD-0234	$C_{13}H_{13}NO_3$	231.2535
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		rotatable bonds
		4.0000
		H-bond acceptors
3.0000		
H-bond donors		
0.0000		
LogP	1.5131	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-(4-oxopentyl)-1H-isoindole-1,3(2H)-dione		

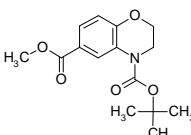
DD-0701	$C_6H_6ClN_3O_2$	187.5866
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		1.0000
		H-bond acceptors
3.0000		
H-bond donors		
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N-(3-chloro-5-nitro-2-pyridinyl)-N-methylamine		

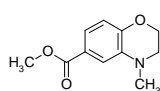
DD-0702	$C_7H_8ClN_3O_2$	201.6137
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		rotatable bonds
		2.0000
		H-bond acceptors
3.0000		
H-bond donors		
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LogP	1.6780	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
N-(3-chloro-5-nitro-2-pyridinyl)-N-ethylamine		

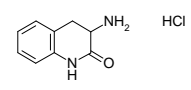
DD-0703	$C_7H_8ClN_3O_3$	217.6131
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		rotatable bonds
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4.0000		
H-bond donors		
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2-[(3-chloro-5-nitro-2-pyridinyl)amino]-1-ethanol		

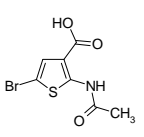
DD-0704	$C_5H_3ClN_2O_2S$	190.6089
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		rotatable bonds
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3.0000		
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LogS	contact Key Organics for details	TPSA contact Key Organics for details
3-chloro-5-nitro-2-pyridinethiol		

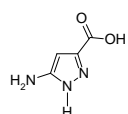
DD-0705	$C_{11}H_{13}NO_5S$	271.2940
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		rotatable bonds
		3.0000
		H-bond acceptors
5.0000		
H-bond donors		
0.0000		
LogP	0.3589	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
methyl 4-(methylsulfonyl)-3,4-dihydro-2H-1,4-benzoxazine-6-carboxylate		

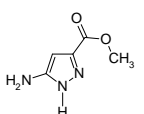
DD-0706	C ₁₅ H ₁₉ NO ₅	293.3224
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	H-bond donors	0.0000
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4-(tert-butyl) 6-methyl 2,3-dihydro-4H-1,4-benzoxazine-4,6-dicarboxylate		

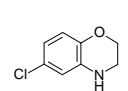
DD-0707	C ₁₁ H ₁₃ NO ₃	207.2312
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	rotatable bonds	2.0000
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methyl 4-methyl-3,4-dihydro-2H-1,4-benzoxazine-6-carboxylate		

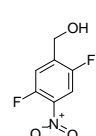
DD-0708	C ₉ H ₁₁ ClN ₂ O	198.6538
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	LogP	0.4776
	LogS	contact Key Organics for details
3-amino-3,4-dihydroquinolin-2(1H)-one hydrochloride		

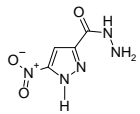
DD-0709	C ₇ H ₆ BrNO ₃ S	264.0988
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	rotatable bonds	2.0000
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	LogP	0.4975
	LogS	contact Key Organics for details
2-(acetylamino)-5-bromo-3-thiophenecarboxylic acid		

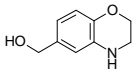
DD-0710	C ₄ H ₅ N ₃ O ₂	127.1034
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	LogP	-0.3690
	LogS	contact Key Organics for details
5-amino-1H-pyrazole-3-carboxylic acid		

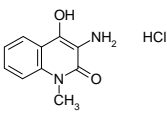
DD-0712	C ₆ H ₇ N ₃ O ₂	141.1304
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	H-bond acceptors	3.0000
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	LogP	-0.3373
	LogS	contact Key Organics for details
methyl 5-amino-1H-pyrazole-3-carboxylate		

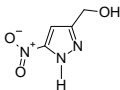
DD-0714	C ₈ H ₈ ClNO	169.6121
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	LogP	1.5647
	LogS	contact Key Organics for details
6-chloro-3,4-dihydro-2H-1,4-benzoxazine		

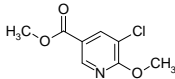
DD-0715	C ₇ H ₅ F ₂ NO ₃	189.1196
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	rotatable bonds	1.0000
	H-bond acceptors	3.0000
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	LogP	1.7439
	LogS	contact Key Organics for details
(2,5-difluoro-4-nitrophenyl)methanol		

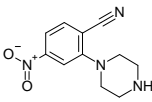
DD-0719	C ₄ H ₅ N ₅ O ₃	171.1162											
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	5.0000												
H-bond donors	3.0000												
LogP	-0.5098												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-nitro-1H-pyrazole-3-carbohydrazide													

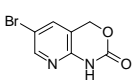
DD-0721	C ₉ H ₁₁ NO ₂	165.1935											
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.5114												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3,4-dihydro-2H-1,4-benzoxazin-6-ylmethanol													

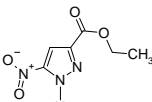
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	-0.8941												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-amino-4-hydroxy-1-methylquinolin-2(1H)-one hydrochloride													


DD-0726	C ₄ H ₅ N ₃ O ₃	143.1028											
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.1341												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(5-nitro-1H-pyrazol-3-yl)methanol													

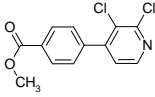
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rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP	1.4287												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 5-chloro-6-methoxynicotinate													

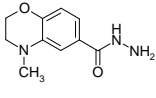
DD-0731	C ₁₁ H ₁₂ N ₄ O ₂	232.2439											
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.0971												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-nitro-2-piperazinobenzecarbonitrile													

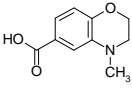
DD-0732	C ₇ H ₅ BrN ₂ O ₂	229.0341											
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.4293												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-bromo-1,4-dihydro-2H-pyrido[2,3-d][1,3]oxazin-2-one													

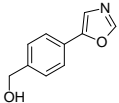
DD-0733	C ₆ H ₇ N ₃ O ₄	185.1404											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	5.0000												
H-bond donors	1.0000												
LogP	0.7420												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 5-nitro-1H-pyrazole-3-carboxylate													

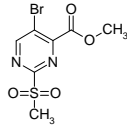
DD-0735	C ₇ H ₄ BrClN ₂	231.4803	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.8477</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	0.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.8477
Halogen atoms	2.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.8477												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-bromo-7-chloro-1H-indazole													

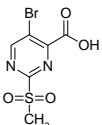
DD-0736	C ₁₃ H ₉ Cl ₂ NO ₂	282.1282	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>4.0208</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	4.0208
Halogen atoms	2.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	4.0208												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 4-(2,3-dichloro-4-pyridinyl)benzenecarboxylate													

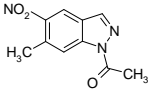
DD-0737	C ₁₀ H ₁₃ N ₃ O ₂	207.2340	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.2289</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	0.2289
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	0.2289												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-methyl-3,4-dihydro-2H-1,4-benzoxazine-6-carbohydrazide													

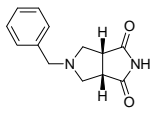
DD-0738	C ₁₀ H ₁₁ NO ₃	193.2041	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.1065</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.1065
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.1065												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-methyl-3,4-dihydro-2H-1,4-benzoxazine-6-carboxylic acid													

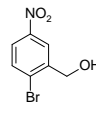
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.3081												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
[4-(1,3-oxazol-5-yl)phenyl]methanol													

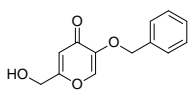
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Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	6.0000												
H-bond donors	0.0000												
LogP	0.6597												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 5-bromo-2-(methylsulfonyl)-4-pyrimidinecarboxylate													

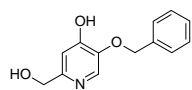
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	6.0000												
H-bond donors	1.0000												
LogP	0.6280												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-bromo-2-(methylsulfonyl)-4-pyrimidinecarboxylic acid													

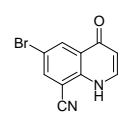
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Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP	1.5593												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(6-methyl-5-nitro-1H-indazol-1-yl)-1-ethanone													

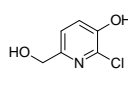
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.5091												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(3aR,6aS)-5-benzyltetrahydropyrrolo[3,4-c]pyrrole-1,3(2H,3aH)-dione													

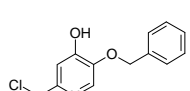
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Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.2567												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(2-bromo-5-nitrophenyl)methanol													

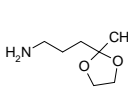
ED-0040	$C_{13}H_{12}O_4$	232.2382											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	-0.3239												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-(benzyloxy)-2-(hydroxymethyl)-4H-pyran-4-one													

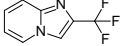
ED-0044	$C_{13}H_{13}NO_3$	231.2535											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	1.8380												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-(benzyloxy)-2-(hydroxymethyl)-4-pyridinol													

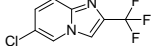
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.6608												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-bromo-4-oxo-1,4-dihydro-8-quinolinecarbonitrile													

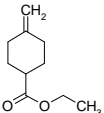
ED-0050	$C_6H_6ClNO_2$	159.5732											
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Halogen atoms	1.0000												
rotatable bonds	1.0000												
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2-chloro-6-(hydroxymethyl)-3-pyridinol													

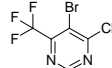
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Halogen atoms	1.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-(benzyloxy)-2-(chloromethyl)-4-pyridinol													

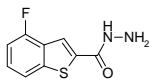
ED-0211	$C_7H_{15}NO_2$	145.2031											
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rotatable bonds	3.0000												
H-bond acceptors	3.0000												
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LogP	0.1424												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(2-methyl-1,3-dioxolan-2-yl)-1-propanamine													

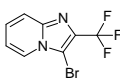
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(trifluoromethyl)imidazo[1,2-a]pyridine													

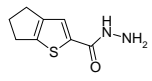
ED-0229	$C_8H_4ClF_3N_2$	220.5827											
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H-bond donors	0.0000												
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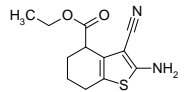
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rotatable bonds	3.0000												
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H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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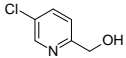
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Halogen atoms	5.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	3.0530												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-bromo-4-chloro-6-(trifluoromethyl)pyrimidine													

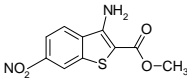
ED-0249	$C_9H_7FN_2OS$	210.2313											
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rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-fluoro-1-benzothiophene-2-carbohydrazide													

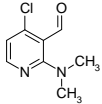
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Halogen atoms	4.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	0.0000												
LogP	2.8722												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-bromo-2-(trifluoromethyl)imidazo[1,2-a]pyridine													

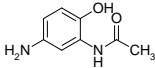
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H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.6054												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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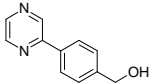
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.1452												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 2-amino-3-cyano-4,5,6,7-tetrahydro-1-benzothiophene-4-carboxylate													

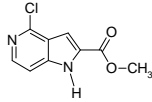
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rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
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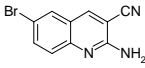
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.0052												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 3-amino-6-nitro-1-benzothiophene-2-carboxylate													

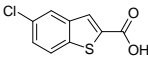
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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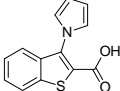
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	3.0000												
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N-(5-amino-2-hydroxyphenyl)acetamide													

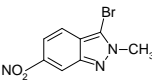
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H-bond donors	1.0000												
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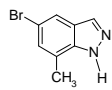
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Halogen atoms	1.0000												
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H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.8909												
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methyl 4-chloro-1H-pyrrolo[3,2-c]pyridine-2-carboxylate													

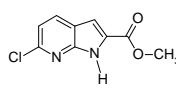
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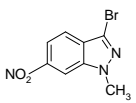
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rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-chloro-1-benzothiophene-2-carboxylic acid													

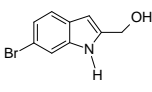
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
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H-bond donors	1.0000												
LogP	2.5632												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(1H-pyrrol-1-yl)-1-benzothiophene-2-carboxylic acid													

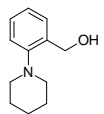
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.4088												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-bromo-2-methyl-6-nitro-2H-indazole													

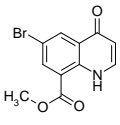
ED-0740	C ₈ H ₇ BrN ₂	211.0624	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.3994</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	0.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.3994
Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.3994												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-bromo-7-methyl-1H-indazole													

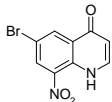
ED-0741	C ₉ H ₇ ClN ₂ O ₂	210.6213	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.6490</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.6490
Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.6490												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 6-chloro-1H-pyrrolo[2,3-b]pyridine-2-carboxylate													

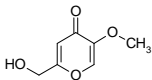
ED-0742	C ₈ H ₆ BrN ₃ O ₂	256.0599	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.5298</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.5298
Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.5298												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-bromo-1-methyl-6-nitro-1H-indazole													

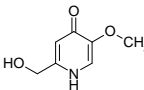
ED-0743	C ₉ H ₈ BrNO	226.0742	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>1.8405</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	1.0000	H-bond acceptors	1.0000	H-bond donors	2.0000	LogP	1.8405
Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	1.0000												
H-bond donors	2.0000												
LogP	1.8405												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(6-bromo-1H-indol-2-yl)methanol													

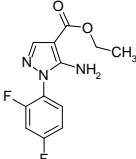
ED-0758	C ₁₂ H ₁₇ NO	191.2754	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.0252</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.0252
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.0252												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(2-piperidinophenyl)methanol													

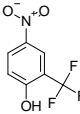
FD-0006	C ₁₁ H ₈ BrNO ₃	282.0953	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.5259</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.5259
Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.5259												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 6-bromo-4-oxo-1,4-dihydro-8-quinolinecarboxylate													

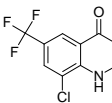
FD-0016	C ₉ H ₅ BrN ₂ O ₃	269.0558	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.7494</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.7494
Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.7494												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-bromo-8-nitro-4(1H)-quinolinone													

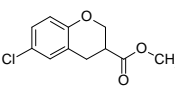
FD-0057	C ₇ H ₈ O ₄	156.1394	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>-2.1005</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	-2.1005
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	-2.1005												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(hydroxymethyl)-5-methoxy-4H-pyran-4-one													

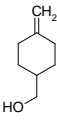
FD-0078	C ₇ H ₉ NO ₃	155.1547	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>-2.4172</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	-2.4172
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	-2.4172												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(hydroxymethyl)-5-methoxy-4(1H)-pyridinone													

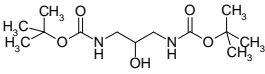
FD-0087	C ₁₂ H ₁₁ F ₂ N ₃ O ₂	267.2372	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.0456</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	4.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.0456
Halogen atoms	2.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.0456												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 5-amino-1-(2,4-difluorophenyl)-1H-pyrazole-4-carboxylate													

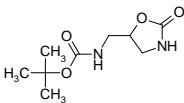
FD-0093	C ₇ H ₄ F ₃ NO ₃	207.1100	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.5986</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.5986
Halogen atoms	3.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.5986												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-nitro-2-(trifluoromethyl)benzenol													

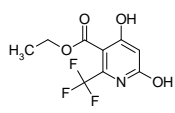
FD-0114	C ₁₀ H ₅ ClF ₃ NO	247.6057	<table border="1"> <tr><td>Halogen atoms</td><td>4.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.4048</td></tr> </table>	Halogen atoms	4.0000	rotatable bonds	0.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.4048
Halogen atoms	4.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.4048												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
8-chloro-6-(trifluoromethyl)-4(1H)-quinolinone													

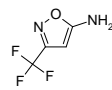
FD-0220	C ₁₁ H ₁₁ ClO ₃	226.6615	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.1960</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.1960
Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.1960												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 6-chloro-3-chromanecarboxylate													

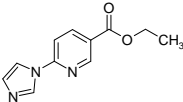
FD-0222	C ₈ H ₁₄ O	126.2002	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.5718</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	1.5718
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	1.5718												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(4-methylenecyclohexyl)methanol													

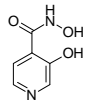
FD-0231	$C_{13}H_{26}N_2O_5$	290.3626	
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		H-bond acceptors	5.0000
		H-bond donors	3.0000
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		LogS	TPSA
contact Key Organics for details contact Key Organics for details tert-butyl N-[(2-hydroxypropyl)amino]carbamate			

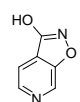
FD-0238	$C_9H_{16}N_2O_4$	216.2389	
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		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	0.2270
		LogS	TPSA
contact Key Organics for details contact Key Organics for details tert-butyl N-[(2-oxo-1,3-oxazolan-5-yl)methyl]carbamate			

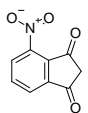
FD-0250	$C_9H_8F_3NO_4$	251.1636	
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		rotatable bonds	3.0000
		H-bond acceptors	5.0000
		H-bond donors	2.0000
		LogP	2.2190
		LogS	TPSA
contact Key Organics for details contact Key Organics for details ethyl 4,6-dihydroxy-2-(trifluoromethyl)nicotinate			

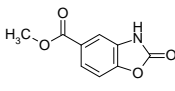
FD-0252	$C_4H_3F_3N_2O$	152.0765	
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		rotatable bonds	0.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	0.9928
		LogS	TPSA
contact Key Organics for details contact Key Organics for details 3-(trifluoromethyl)-5-isoxazolamine			

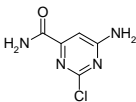
FD-0707	$C_{11}H_{11}N_3O_2$	217.2292	
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		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
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		LogS	TPSA
contact Key Organics for details contact Key Organics for details ethyl 6-(1H-imidazol-1-yl)nicotinate			

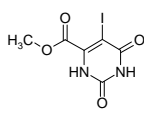
FD-0713	$C_6H_6N_2O_3$	154.1263	
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		LogP	0.2348
		LogS	TPSA
contact Key Organics for details contact Key Organics for details N,3-dihydroxyisonicotinamide			

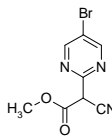
FD-0722	$C_6H_4N_2O_2$	136.1110	
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		rotatable bonds	0.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
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		LogS	TPSA
contact Key Organics for details contact Key Organics for details isoxazolo[5,4-c]pyridin-3-ol			

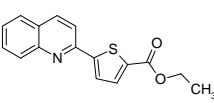
FD-0726	$C_6H_5NO_4$	191.1445	
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		rotatable bonds	0.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	0.6445
		LogS	TPSA
contact Key Organics for details contact Key Organics for details 4-nitro-1H-indene-1,3(2H)-dione			

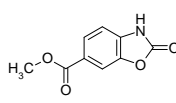
FD-0728	C ₉ H ₇ NO ₄	193.1604	
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			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
4.0000			
H-bond donors	1.0000		
LogP	0.5362		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-oxo-2,3-dihydro-1,3-benzoxazole-5-carboxylate			

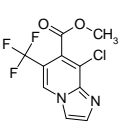
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			rotatable bonds
			1.0000
			H-bond acceptors
3.0000			
H-bond donors	2.0000		
LogP	-0.0681		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
6-amino-2-chloro-4-pyrimidinecarboxamide			

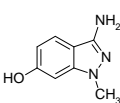
FD-0731	C ₆ H ₅ I ₂ N ₂ O ₄	296.0222	
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			1.0000
			rotatable bonds
			2.0000
			H-bond acceptors
4.0000			
H-bond donors	2.0000		
LogP	-1.1570		
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methyl 5-iodo-2,6-dioxo-1,2,3,6-tetrahydro-4-pyrimidinecarboxylate			

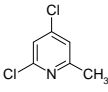
FD-0732	C ₈ H ₆ BrN ₃ O ₂	256.0599	
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			1.0000
			rotatable bonds
			3.0000
			H-bond acceptors
5.0000			
H-bond donors	0.0000		
LogP	1.1677		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-(5-bromo-2-pyrimidinyl)-2-cyanoacetate			


FD-0734	C ₁₆ H ₁₃ NO ₂ S	283.3515	
			Halogen atoms
			0.0000
			rotatable bonds
			4.0000
			H-bond acceptors
3.0000			
H-bond donors	0.0000		
LogP	3.3480		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 5-(2-quinolinyl)-2-thiophenecarboxylate			

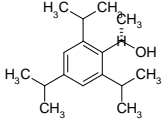
FD-0742	C ₉ H ₇ NO ₄	193.1604	
			Halogen atoms
			0.0000
			rotatable bonds
			2.0000
			H-bond acceptors
4.0000			
H-bond donors	1.0000		
LogP	0.5362		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-oxo-2,3-dihydro-1,3-benzoxazole-6-carboxylate			

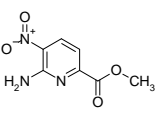
FD-0745	C ₁₀ H ₆ ClF ₃ N ₂ O ₂	278.6197	
			Halogen atoms
			4.0000
			rotatable bonds
			2.0000
			H-bond acceptors
3.0000			
H-bond donors	0.0000		
LogP	1.3845		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 8-chloro-6-(trifluoromethyl)imidazo[1,2-a]pyridine-7-carboxylate			

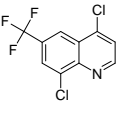
FD-0747	C ₈ H ₉ N ₃ O	163.1804	
			Halogen atoms
			0.0000
			rotatable bonds
			0.0000
			H-bond acceptors
2.0000			
H-bond donors	2.0000		
LogP	1.0179		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-amino-1-methyl-1H-indazol-6-ol			

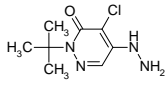
FD-0748	$C_6H_5Cl_2N$	162.0195
		Halogen atoms 2.0000
		rotatable bonds 0.0000
		H-bond acceptors 1.0000
		H-bond donors 0.0000
		LogP 2.7908
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2,4-dichloro-6-methylpyridine		

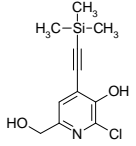
FD-0749	$C_7H_6N_2S$	150.2033
		Halogen atoms 0.0000
		rotatable bonds 0.0000
		H-bond acceptors 1.0000
		H-bond donors 1.0000
		LogP 1.0035
LogS	contact Key Organics for details	TPSA contact Key Organics for details
thieno[2,3-b]pyridin-3-ylamine		

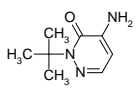
FS-0002	$C_{17}H_{28}O$	248.4121
		Halogen atoms 0.0000
		rotatable bonds 4.0000
		H-bond acceptors 1.0000
		H-bond donors 1.0000
		LogP 5.5064
LogS	contact Key Organics for details	TPSA contact Key Organics for details
(S)-(-)-STERICOL		

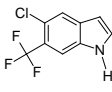
GA-0750	$C_7H_7N_3O_4$	197.1515
		Halogen atoms 0.0000
		rotatable bonds 2.0000
		H-bond acceptors 5.0000
		H-bond donors 1.0000
		LogP 0.7329
LogS	contact Key Organics for details	TPSA contact Key Organics for details
methyl 6-amino-5-nitro-2-pyridinecarboxylate		

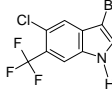
GD-0001	$C_{10}H_4Cl_2F_3N$	266.0513
		Halogen atoms 5.0000
		rotatable bonds 0.0000
		H-bond acceptors 1.0000
		H-bond donors 0.0000
		LogP 4.0548
LogS	contact Key Organics for details	TPSA contact Key Organics for details
4,8-dichloro-6-(trifluoromethyl)quinoline		

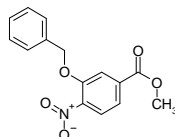
GD-0003	$C_8H_{13}ClN_4O$	216.6720
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		rotatable bonds 2.0000
		H-bond acceptors 3.0000
		H-bond donors 2.0000
		LogP
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-(tert-butyl)-4-chloro-5-hydrazino-3(2H)-pyridazinone		

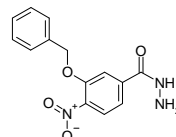
GD-0009	$C_{11}H_{14}ClNO_2Si$	255.7787
		Halogen atoms 1.0000
		rotatable bonds 4.0000
		H-bond acceptors 3.0000
		H-bond donors 2.0000
		LogP
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-chloro-6-methoxy-4-[2-(trimethylsilyl)ethynyl]-3-pyridinol		

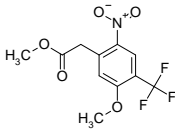
GD-0015	$C_8H_{13}N_3O$	167.2123
		Halogen atoms 0.0000
		rotatable bonds 1.0000
		H-bond acceptors 2.0000
		H-bond donors 1.0000
		LogP -0.5352
LogS	contact Key Organics for details	TPSA contact Key Organics for details
4-amino-2-(tert-butyl)-3(2H)-pyridazinone		

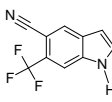
GD-0016	C ₉ H ₅ ClF ₃ N	219.5951	<table border="1"> <tr><td>Halogen atoms</td><td>4.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>0.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>3.2206</td></tr> </table>	Halogen atoms	4.0000	rotatable bonds	0.0000	H-bond acceptors	0.0000	H-bond donors	1.0000	LogP	3.2206
Halogen atoms	4.0000												
rotatable bonds	0.0000												
H-bond acceptors	0.0000												
H-bond donors	1.0000												
LogP	3.2206												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-chloro-6-(trifluoromethyl)-1H-indole													

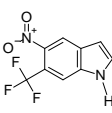
GD-0025	C ₉ H ₄ BrClF ₃ N	298.4911	<table border="1"> <tr><td>Halogen atoms</td><td>5.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>0.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>4.0124</td></tr> </table>	Halogen atoms	5.0000	rotatable bonds	0.0000	H-bond acceptors	0.0000	H-bond donors	1.0000	LogP	4.0124
Halogen atoms	5.0000												
rotatable bonds	0.0000												
H-bond acceptors	0.0000												
H-bond donors	1.0000												
LogP	4.0124												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-bromo-5-chloro-6-(trifluoromethyl)-1H-indole													

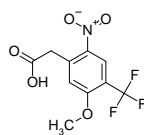
GD-0029	C ₁₅ H ₁₃ NO ₅	287.2746	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>5.0000</td></tr> <tr><td>H-bond acceptors</td><td>5.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>3.2542</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	5.0000	H-bond acceptors	5.0000	H-bond donors	0.0000	LogP	3.2542
Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	5.0000												
H-bond donors	0.0000												
LogP	3.2542												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 3-(benzyloxy)-4-nitrobenzenecarboxylate													

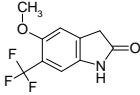
GD-0052	C ₁₄ H ₁₃ N ₃ O ₄	287.2774	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>5.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>2.3449</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	5.0000	H-bond donors	2.0000	LogP	2.3449
Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	5.0000												
H-bond donors	2.0000												
LogP	2.3449												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(benzyloxy)-4-nitrobenzenecarbohydrazide													

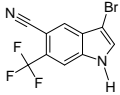
GD-0054	C ₁₁ H ₁₀ F ₃ NO ₅	293.2013	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>5.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.2929</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	4.0000	H-bond acceptors	5.0000	H-bond donors	0.0000	LogP	2.2929
Halogen atoms	3.0000												
rotatable bonds	4.0000												
H-bond acceptors	5.0000												
H-bond donors	0.0000												
LogP	2.2929												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 2-[5-methoxy-2-nitro-4-(trifluoromethyl)phenyl]acetate													

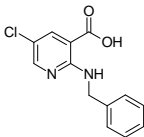
GD-0077	C ₁₀ H ₅ F ₃ N ₂	210.1599	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.5676</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	0.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.5676
Halogen atoms	3.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.5676												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-(trifluoromethyl)-1H-indole-5-carbonitrile													

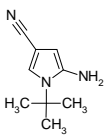
GD-0078	C ₉ H ₅ F ₃ N ₂ O ₂	230.1476	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.6562</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	0.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	2.6562
Halogen atoms	3.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.6562												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-nitro-6-(trifluoromethyl)-1H-indole													

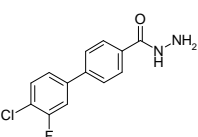
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Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	5.0000												
H-bond donors	1.0000												
LogP	2.2612												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[5-methoxy-2-nitro-4-(trifluoromethyl)phenyl]acetic acid													

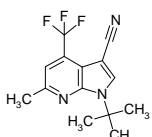
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.1495												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-methoxy-6-(trifluoromethyl)-1,3-dihydro-2H-indol-2-one													

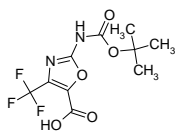
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Halogen atoms	4.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	3.3594												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-bromo-6-(trifluoromethyl)-1H-indole-5-carbonitrile													

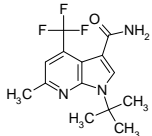
GD-0094	C ₁₃ H ₁₁ ClN ₂ O ₂	262.6978	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>3.3218</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	4.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	3.3218
Halogen atoms	1.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	3.3218												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(benzylamino)-5-chloronicotinic acid													

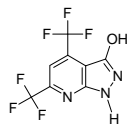
GD-0202	C ₉ H ₁₃ N ₃	163.2241	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.1582</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	1.1582
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	1.1582												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-amino-1-(tert-butyl)-1H-pyrrole-3-carbonitrile													

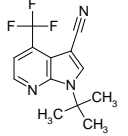
GD-0207	C ₁₃ H ₁₀ ClFN ₂ O	264.6889	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>3.2093</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	3.2093
Halogen atoms	2.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	3.2093												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4'-chloro-3'-fluoro[1,1'-biphenyl]-4-carbohydrazide													

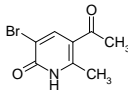
GD-0209	C ₁₄ H ₁₄ F ₃ N ₃	281.2830	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>3.7435</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	1.0000	H-bond acceptors	2.0000	H-bond donors	0.0000	LogP	3.7435
Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	3.7435												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(tert-butyl)-6-methyl-4-(trifluoromethyl)-1H-pyrrolo[2,3-b]pyridine-3-carbonitrile													

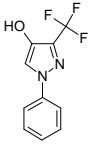
GD-0210	C ₁₀ H ₁₁ F ₃ N ₂ O ₅	296.2048	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>6.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>1.8919</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	4.0000	H-bond acceptors	6.0000	H-bond donors	2.0000	LogP	1.8919
Halogen atoms	3.0000												
rotatable bonds	4.0000												
H-bond acceptors	6.0000												
H-bond donors	2.0000												
LogP	1.8919												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[(tert-butoxycarbonyl)amino]-4-(trifluoromethyl)-1,3-oxazole-5-carboxylic acid													

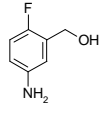
GD-0220	C ₁₄ H ₁₆ F ₃ N ₃ O	299.2983	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.7121</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	2.7121
Halogen atoms	3.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.7121												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(tert-butyl)-6-methyl-4-(trifluoromethyl)-1H-pyrrolo[2,3-b]pyridine-3-carboxamide													

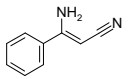
GD-0225	$C_8H_3F_6N_3O$	271.1230											
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Halogen atoms	6.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	3.1655												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4,6-bis(trifluoromethyl)-1H-pyrazolo[3,4-b]pyridin-3-ol													

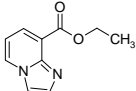
GD-0240	$C_{13}H_{12}F_3N_3$	267.2559											
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rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	3.0941												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(tert-butyl)-4-(trifluoromethyl)-1H-pyrrolo[2,3-b]pyridine-3-carbonitrile													


GD-0241	$C_8H_8BrNO_2$	230.0625											
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rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	-1.3022												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-acetyl-3-bromo-6-methyl-2(1H)-pyridinone													

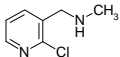
GD-0702	$C_{10}H_7F_3N_2O$	228.1753											
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	3.5320												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-phenyl-3-(trifluoromethyl)-1H-pyrazol-4-ol													

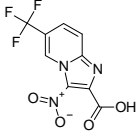
GD-0704	C_7H_8FNO	141.1463											
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Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	1.0000												
H-bond donors	2.0000												
LogP	0.8676												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(5-amino-2-fluorophenyl)methanol													

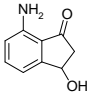
GD-0705	$C_9H_8N_2$	144.1775											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	0.6013												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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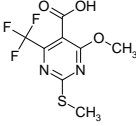
GD-0707	$C_{10}H_{10}N_2O_2$	190.2034											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	1.3806												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl imidazo[1,2-a]pyridine-8-carboxylate													

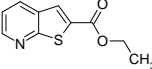
GD-0711	$C_6H_8N_2O_2$	140.1429											
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Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	-0.6245												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2,4-diazabicyclo[4.2.0]octane-3,5-dione													


GD-0716	C ₇ H ₉ ClN ₂	156.6162	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.1489</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	1.1489
Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.1489												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>(2-chloro-3-pyridinyl)-N-methylmethanamine</p>													

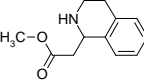
GD-0717	C ₉ H ₄ F ₃ N ₃ O ₄	275.1451	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>5.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.7197</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	1.0000	H-bond acceptors	5.0000	H-bond donors	1.0000	LogP	1.7197
Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	5.0000												
H-bond donors	1.0000												
LogP	1.7197												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>3-nitro-6-(trifluoromethyl)imidazo[1,2-a]pyridine-2-carboxylic acid</p>													

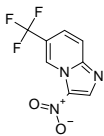
GD-0718	C ₉ H ₉ NO ₂	163.1776	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>-0.0018</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	0.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	-0.0018
Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	-0.0018												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>7-amino-3-hydroxy-1-indanone</p>													

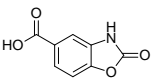
GD-0719	C ₈ H ₇ F ₃ N ₂ O ₃ S	268.2158	<table border="1"> <tr><td>Halogen atoms</td><td>3.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>5.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.1105</td></tr> </table>	Halogen atoms	3.0000	rotatable bonds	3.0000	H-bond acceptors	5.0000	H-bond donors	1.0000	LogP	2.1105
Halogen atoms	3.0000												
rotatable bonds	3.0000												
H-bond acceptors	5.0000												
H-bond donors	1.0000												
LogP	2.1105												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>4-methoxy-2-(methylsulfanyl)-6-(trifluoromethyl)-5-pyrimidinecarboxylic acid</p>													

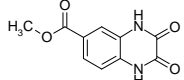
GD-0724	C ₁₀ H ₉ NO ₂ S	207.2527	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.0884</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.0884
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.0884												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>ethyl thieno[2,3-b]pyridine-2-carboxylate</p>													

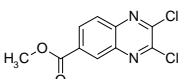
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.1102												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>(2-methoxy-3-pyridinyl)methanol</p>													

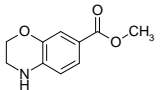
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.3792												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>methyl 2-(1,2,3,4-tetrahydro-1-isoquinolinyl)acetate</p>													

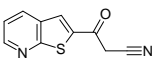
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Halogen atoms	3.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.0871												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
<p>3-nitro-6-(trifluoromethyl)imidazo[1,2-a]pyridine</p>													

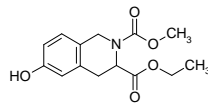
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.5045												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-oxo-2,3-dihydro-1,3-benzoxazole-5-carboxylic acid													

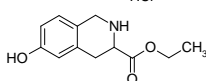
GD-0747	$C_{10}H_8N_2O_4$	220.1863	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>-0.4307</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	2.0000	LogP	-0.4307
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	-0.4307												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 2,3-dioxo-1,2,3,4-tetrahydro-6-quinoxalinecarboxylate													

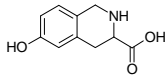
GD-0751	$C_{10}H_6Cl_2N_2O_2$	257.0775	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.7307</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	0.0000	LogP	2.7307
Halogen atoms	2.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP	2.7307												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 2,3-dichloro-6-quinoxalinecarboxylate													

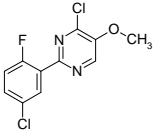
GD-0753	$C_{10}H_{11}NO_3$	193.2041	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.7768</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	0.7768
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.7768												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 3,4-dihydro-2H-1,4-benzoxazine-7-carboxylate													

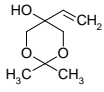
GD-0761	$C_{10}H_6N_2OS$	202.2361	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>0.8854</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	0.8854
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	0.8854												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-oxo-3-thieno[2,3-b]pyridin-2-ylpropanenitrile													

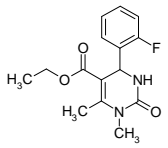
H-20039	$C_{14}H_{17}NO_5$	279.2953	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>5.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.6705</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	5.0000	H-bond donors	1.0000	LogP	1.6705
Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	5.0000												
H-bond donors	1.0000												
LogP	1.6705												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-ethyl 2-methyl 6-hydroxy-3,4-dihydro-2,3(1H)-isoquinolinedicarboxylate													

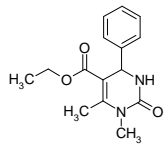
H-20242	$C_{12}H_{16}ClNO_3$	257.7192	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>1.6889</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	1.0000	H-bond acceptors	4.0000	H-bond donors	2.0000	LogP	1.6889
Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	1.6889												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 6-hydroxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylate hydrochloride													

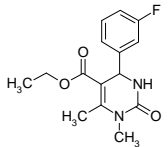
H-20243	$C_{10}H_{11}NO_3$	193.2041	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>3.0000</td></tr> <tr><td>LogP</td><td>1.0062</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	4.0000	H-bond donors	3.0000	LogP	1.0062
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	3.0000												
LogP	1.0062												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-hydroxy-1,2,3,4-tetrahydro-3-isoquinolinecarboxylic acid													

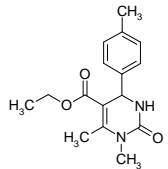
H-20257	C ₁₁ H ₇ Cl ₂ FN ₂ O	273.0956	
		Halogen atoms	3.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	3.2661
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-chloro-2-(5-chloro-2-fluorophenyl)-5-methoxypyrimidine			

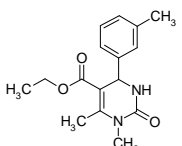
H-20267	C ₈ H ₁₄ O ₃	158.1990	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.7761
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
2,2-dimethyl-5-vinyl-1,3-dioxan-5-ol			

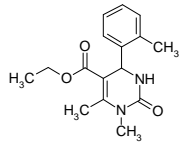
HA-0232	C ₁₅ H ₁₇ FN ₂ O ₃	292.3127	
		Halogen atoms	1.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.9505
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 4-(2-fluorophenyl)-1,6-dimethyl-2-oxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

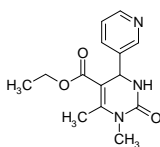
HA-0233	C ₁₅ H ₁₈ N ₂ O ₃	274.3223	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.8110
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 1,6-dimethyl-2-oxo-4-phenyl-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

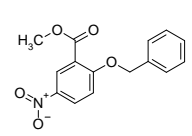
HA-0237	C ₁₅ H ₁₇ FN ₂ O ₃	292.3127	
		Halogen atoms	1.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.9505
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 4-(3-fluorophenyl)-1,6-dimethyl-2-oxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

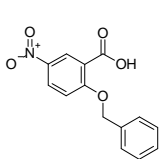
HA-0240	C ₁₆ H ₂₀ N ₂ O ₃	288.3494	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.2782
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 1,6-dimethyl-4-(4-methylphenyl)-2-oxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

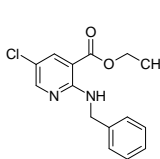
HA-0242	C ₁₆ H ₂₀ N ₂ O ₃	288.3494	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.2782
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 1,6-dimethyl-4-(3-methylphenyl)-2-oxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

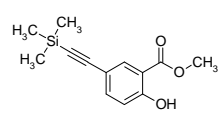
HA-0244	C ₁₆ H ₂₀ N ₂ O ₃	288.3494	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.2782
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 1,6-dimethyl-4-(2-methylphenyl)-2-oxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

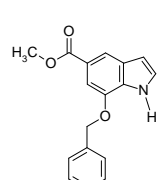
HA-0247	C ₁₄ H ₁₇ N ₃ O ₃	275.3099	
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		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	-0.0360
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 1,6-dimethyl-2-oxo-4-(3-pyridinyl)-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate			

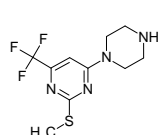
HD-0002	C ₁₅ H ₁₃ NO ₅	287.2746	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	3.2542
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-(benzyloxy)-5-nitrobenzenecarboxylate			

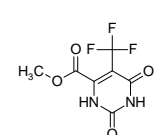
HD-0007	C ₁₄ H ₁₁ NO ₅	273.2475	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	5.0000
		H-bond donors	1.0000
		LogP	3.2225
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
2-(benzyloxy)-5-nitrobenzenecarboxylic acid			

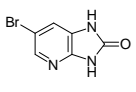
HD-0026	C ₁₅ H ₁₅ ClN ₂ O ₂	290.7520	
		Halogen atoms	1.0000
		rotatable bonds	6.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	3.6960
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 2-(benzylamino)-5-chloronicotinate			

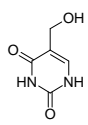
HD-0078	C ₁₃ H ₁₆ O ₃ Si	248.3567	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2-hydroxy-5-[2-(trimethylsilyl)ethynyl]benzenecarboxylate			

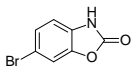
HD-0094	C ₁₇ H ₁₅ NO ₃	281.3140	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	3.0738
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 7-(benzyloxy)-1H-indole-5-carboxylate			

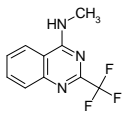
HD-0233	C ₁₀ H ₁₃ F ₃ N ₄ S	278.3011	
		Halogen atoms	3.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.8967
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
2-(methylsulfanyl)-4-piperazino-6-(trifluoromethyl)pyrimidine			

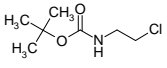
HD-0237	C ₇ H ₅ F ₃ N ₂ O ₄	238.1241	
		Halogen atoms	3.0000
		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	-1.1048
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 2,6-dioxo-5-(trifluoromethyl)-1,2,3,6-tetrahydro-4-pyrimidinecarboxylate			

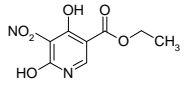
HD-0706	C ₆ H ₄ BrN ₃ O	214.0223
		Halogen atoms 1.0000
		rotatable bonds 0.0000
		H-bond acceptors 2.0000
		H-bond donors 2.0000
		LogP -0.0187
LogS	contact Key Organics for details	TPSA contact Key Organics for details
6-bromo-1,3-dihydro-2H-imidazo[4,5-b]pyridin-2-one		

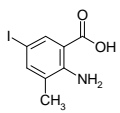
HD-0707	C ₅ H ₆ N ₂ O ₃	142.1152
		Halogen atoms 0.0000
		rotatable bonds 1.0000
		H-bond acceptors 3.0000
		H-bond donors 3.0000
		LogP -1.5657
LogS	contact Key Organics for details	TPSA contact Key Organics for details
5-(hydroxymethyl)-2,4(1H,3H)-pyrimidinedione		


HD-0708	C ₇ H ₄ BrNO ₂	214.0194
		Halogen atoms 1.0000
		rotatable bonds 0.0000
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		H-bond donors 1.0000
		LogP 1.5979
LogS	contact Key Organics for details	TPSA contact Key Organics for details
6-bromo-1,3-benzoxazol-2(3H)-one		

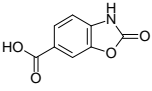
HD-0716	C ₁₀ H ₈ F ₃ N ₃	227.1906
		Halogen atoms 3.0000
		rotatable bonds 1.0000
		H-bond acceptors 2.0000
		H-bond donors 1.0000
		LogP 2.7015
LogS	contact Key Organics for details	TPSA contact Key Organics for details
N-methyl-2-(trifluoromethyl)-4-quinazolinamine		

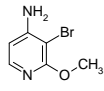
HD-0717	C ₇ H ₁₄ ClNO ₂	179.6481
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		rotatable bonds 4.0000
		H-bond acceptors 2.0000
		H-bond donors 1.0000
		LogP 1.3765
LogS	contact Key Organics for details	TPSA contact Key Organics for details
tert-butyl N-(2-chloroethyl)carbamate		

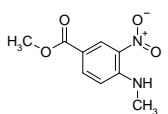
HD-0719	C ₈ H ₈ N ₂ O ₆	228.1628
		Halogen atoms 0.0000
		rotatable bonds 3.0000
		H-bond acceptors 7.0000
		H-bond donors 2.0000
		LogP 0.8907
LogS	contact Key Organics for details	TPSA contact Key Organics for details
ethyl 4,6-dihydroxy-5-nitrocinotinate		

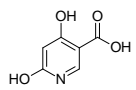
HD-0722	C ₈ H ₈ INO ₂	277.0629
		Halogen atoms 1.0000
		rotatable bonds 1.0000
		H-bond acceptors 2.0000
		H-bond donors 2.0000
		LogP 2.6864
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-amino-5-iodo-3-methylbenzenecarboxylic acid		

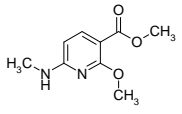
HD-0725	C ₆ H ₇ NO ₂	125.1282
		Halogen atoms 0.0000
		rotatable bonds 0.0000
		H-bond acceptors 2.0000
		H-bond donors 1.0000
		LogP -0.4540
LogS	contact Key Organics for details	TPSA contact Key Organics for details
3-azabicyclo[3.2.0]heptane-2,4-dione		

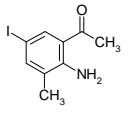
HD-0726	C ₈ H ₅ NO ₄	179.1334	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	0.5045
		LogS	contact Key Organics for details
2-oxo-2,3-dihydro-1,3-benzoxazole-6-carboxylic acid			

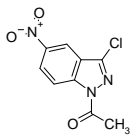
HD-0734	C ₆ H ₇ BrN ₂ O	203.0395	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	1.1892
		LogS	contact Key Organics for details
3-bromo-2-methoxy-4-pyridinamine			

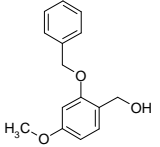
HD-0736	C ₉ H ₁₀ N ₂ O ₄	210.1911	
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		rotatable bonds	3.0000
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		LogP	1.1609
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methyl 4-(methylamino)-3-nitrobenzenecarboxylate			

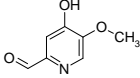
HD-0738	C ₆ H ₅ NO ₄	155.1111	
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		rotatable bonds	1.0000
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		H-bond donors	3.0000
		LogP	0.5629
		LogS	contact Key Organics for details
4,6-dihydroxynicotinic acid			

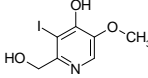
HD-0744	C ₉ H ₁₂ N ₂ O ₃	196.2076	
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		rotatable bonds	4.0000
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		LogP	1.0399
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methyl 2-methoxy-6-(methylamino)nicotinate			

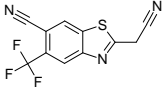
HD-0746	C ₉ H ₁₀ INO	275.0906	
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		rotatable bonds	1.0000
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	2.2965
		LogS	contact Key Organics for details
1-(2-amino-5-iodo-3-methylphenyl)-1-ethanone			

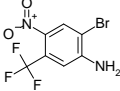
HD-0747	C ₉ H ₆ ClN ₃ O ₃	239.6195	
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		rotatable bonds	0.0000
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		H-bond donors	0.0000
		LogP	1.9808
		LogS	contact Key Organics for details
1-(3-chloro-5-nitro-1H-indazol-1-yl)-1-ethanone			

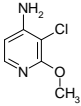
KD-0008	C ₁₅ H ₁₆ O ₃	244.2930	
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		rotatable bonds	5.0000
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		LogP	2.7825
		LogS	contact Key Organics for details
[2-(benzyloxy)-4-methoxyphenyl]methanol			

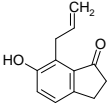
KD-0031	C ₇ H ₇ NO ₃	153.1387											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	0.7371												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-hydroxy-5-methoxy-2-pyridinecarbaldehyde													


KD-0032	C ₇ H ₈ INO ₃	281.0511											
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	1.7837												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(hydroxymethyl)-3-iodo-5-methoxy-4-pyridinol													

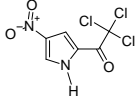
KD-0034	C ₁₁ H ₄ F ₃ N ₃ S	267.2338											
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.4953												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(cyanomethyl)-5-(trifluoromethyl)-1,3-benzothiazole-6-carbonitrile													

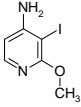
KD-0061	C ₇ H ₄ BrF ₃ N ₂ O ₂	285.0213											
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Halogen atoms	4.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.8916												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-bromo-4-nitro-5-(trifluoromethyl)aniline													


KD-0200	C ₆ H ₇ ClN ₂ O	158.5885											
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Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	0.9154												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-chloro-2-methoxy-4-pyridinamine													

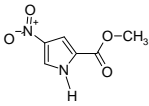
KD-0202	C ₁₂ H ₁₂ O ₂	188.2282											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.3105												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
7-allyl-6-hydroxy-1-indanone													

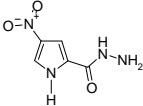
KD-0203	C ₇ H ₆ ClN ₃	167.5990											
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	2.0000												
LogP	1.5738												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
7-chloro-1H-indazol-3-amine													


KD-0208	C ₆ H ₃ Cl ₃ N ₂ O ₃	257.4614											
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.7502												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2,2,2-trichloro-1-(4-nitro-1H-pyrrol-2-yl)-1-ethanone													

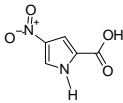
KD-0216	C ₆ H ₇ IN ₂ O	250.0399	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.6548</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	1.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	1.6548
Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.6548												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-iodo-2-methoxy-4-pyridinamine													

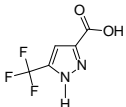
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Halogen atoms	1.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	1.7920												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-(chloromethyl)-2-methoxypyridine													

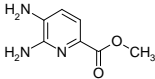
KD-0219	C ₆ H ₆ N ₂ O ₄	170.1257	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.5013</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	0.5013
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	0.5013												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 4-nitro-1H-pyrrole-2-carboxylate													

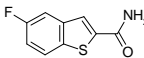
KD-0222	C ₅ H ₆ N ₄ O ₃	170.1286	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>3.0000</td></tr> <tr><td>LogP</td><td>-0.4080</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	4.0000	H-bond donors	3.0000	LogP	-0.4080
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	3.0000												
LogP	-0.4080												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-nitro-1H-pyrrole-2-carbohydrazide													

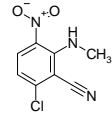
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Halogen atoms	2.0000												
rotatable bonds	0.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	1.3582												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2,3-dichloro-4-pyridinamine													

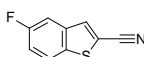
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.4696												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-nitro-1H-pyrrole-2-carboxylic acid													

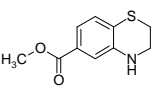
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Halogen atoms	3.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	1.1185												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-(trifluoromethyl)-1H-pyrazole-3-carboxylic acid													

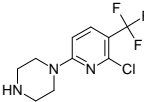
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	-0.0039												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 5,6-diamino-2-pyridinecarboxylate													

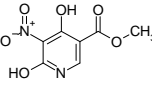
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contact Key Organics for details		contact Key Organics for details	
5-fluoro-1-benzothiophene-2-carboxamide			

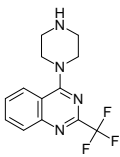
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		H-bond donors	1.0000
		LogP	1.8138
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
6-chloro-2-(methylamino)-3-nitrobenzencarbonitrile			

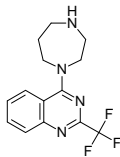
KD-0707	C ₉ H ₄ FNS	177.2013	
		Halogen atoms	1.0000
		rotatable bonds	0.0000
		H-bond acceptors	1.0000
		H-bond donors	0.0000
		LogP	2.1092
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
5-fluoro-1-benzothiophene-2-carbonitrile			

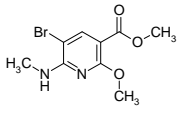
KD-0712	C ₁₀ H ₁₁ NO ₂ S	209.2687	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	1.1201
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
methyl 3,4-dihydro-2H-1,4-benzothiazine-6-carboxylate			

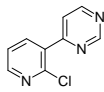
KD-0713	C ₁₀ H ₁₁ ClF ₃ N ₃	265.6675	
		Halogen atoms	4.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	2.4367
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
1-[6-chloro-5-(trifluoromethyl)-2-pyridinyl]piperazine			

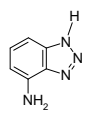
KD-0715	C ₇ H ₆ N ₂ O ₆	214.1357	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	7.0000
		H-bond donors	2.0000
		LogP	1.0131
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
methyl 4,6-dihydroxy-5-nitronicotinate			

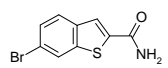
KD-0717	C ₁₃ H ₁₃ F ₃ N ₄	282.2706	
		Halogen atoms	3.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.5028
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
4-piperazino-2-(trifluoromethyl)quinazoline			

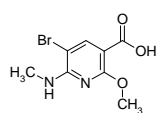
KD-0718	C ₁₄ H ₁₅ F ₃ N ₄	296.2977	
		Halogen atoms	3.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.5549
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
4-(1,4-diazepan-1-yl)-2-(trifluoromethyl)quinazoline			

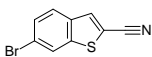
KD-0719	$C_9H_{11}BrN_2O_3$	275.1036
		Halogen atoms
		1.0000
		rotatable bonds
		4.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	1.8317	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
methyl 5-bromo-2-methoxy-6-(methylamino)nicotinate		

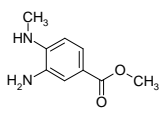
KD-0721	$C_9H_6ClN_3$	191.6213
		Halogen atoms
		1.0000
		rotatable bonds
		1.0000
		H-bond acceptors
		3.0000
H-bond donors		
0.0000		
LogP	1.7509	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
4-(2-chloro-3-pyridinyl)pyrimidine		

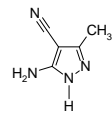
KD-0722	$C_6H_6N_4$	134.1415
		Halogen atoms
		0.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		2.0000
H-bond donors		
2.0000		
LogP	0.3046	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
1H-1,2,3-benzotriazol-4-amine		

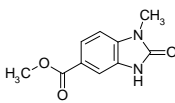
KD-0724	C_9H_6BrNOS	256.1223
		Halogen atoms
		1.0000
		rotatable bonds
		1.0000
		H-bond acceptors
		1.0000
H-bond donors		
1.0000		
LogP	1.7301	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
6-bromo-1-benzothiophene-2-carboxamide		

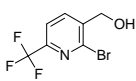
KD-0727	$C_8H_9BrN_2O_3$	261.0765
		Halogen atoms
		1.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		4.0000
H-bond donors		
2.0000		
LogP	1.8000	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
5-bromo-2-methoxy-6-(methylamino)nicotinic acid		

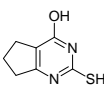
KD-0728	C_9H_4BrNS	238.1069
		Halogen atoms
		1.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		1.0000
H-bond donors		
0.0000		
LogP	2.7615	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
6-bromo-1-benzothiophene-2-carbonitrile		

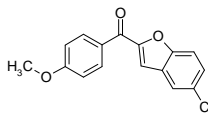
KD-0729	$C_9H_{12}N_2O_2$	180.2082
		Halogen atoms
		0.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		2.0000
H-bond donors		
2.0000		
LogP	0.4241	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
methyl 3-amino-4-(methylamino)benzenecarboxylate		

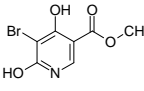
KD-0730	$C_5H_6N_4$	122.1304
		Halogen atoms
		0.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		2.0000
H-bond donors		
2.0000		
LogP	0.0479	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		
5-amino-3-methyl-1H-pyrazole-4-carbonitrile		

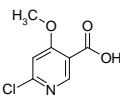
KD-0732	C ₁₀ H ₁₀ N ₂ O ₃	206.2028
		Halogen atoms
		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	0.1327	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
methyl 1-methyl-2-oxo-2,3-dihydro-1H-1,3-benzimidazole-5-carboxylate		

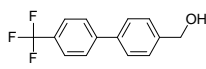
KD-0734	C ₇ H ₅ BrF ₃ NO	256.0232
		Halogen atoms
		4.0000
		rotatable bonds
		1.0000
		H-bond acceptors
		2.0000
H-bond donors		
1.0000		
LogP	2.6706	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
[2-bromo-6-(trifluoromethyl)-3-pyridinyl]methanol		

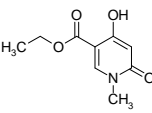
KD-0735	C ₇ H ₈ N ₂ OS	168.2186
		Halogen atoms
		0.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		3.0000
H-bond donors		
2.0000		
LogP	2.0455	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-sulfanyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-ol		

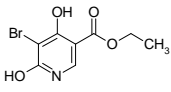
KD-0736	C ₁₆ H ₁₁ ClO ₃	286.7173
		Halogen atoms
		1.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
0.0000		
LogP	3.2481	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
(5-chloro-1-benzofuran-2-yl)(4-methoxyphenyl)methanone		

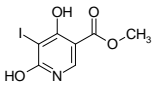
KD-0737	C ₇ H ₆ BrNO ₄	248.0342
		Halogen atoms
		1.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		5.0000
H-bond donors		
2.0000		
LogP	1.8513	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
methyl 5-bromo-4,6-dihydroxynicotinate		

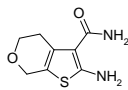
KD-0738	C ₇ H ₆ ClNO ₃	187.5838
		Halogen atoms
		1.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	1.5340	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
6-chloro-4-methoxynicotinic acid		

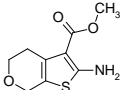
KD-0742	C ₁₄ H ₁₁ F ₃ O	252.2384
		Halogen atoms
		3.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		1.0000
H-bond donors		
1.0000		
LogP	4.0785	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
[4'-(trifluoromethyl)][1,1'-biphenyl]-4-yl]methanol		

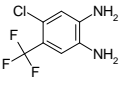
KD-0744	C ₉ H ₁₁ NO ₄	197.1923
		Halogen atoms
		0.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	-1.0552	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
ethyl 4-hydroxy-1-methyl-6-oxo-1,6-dihydro-3-pyridinecarboxylate		


KD-0745	$C_8H_8BrNO_4$	262.0613
		Halogen atoms
		1.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		5.0000
H-bond donors		
2.0000		
LogP	2.1938	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
ethyl 5-bromo-4,6-dihydroxynicotinate		

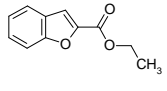
KD-0748	$C_7H_6INO_4$	295.0346
		Halogen atoms
		1.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		5.0000
H-bond donors		
2.0000		
LogP	2.3169	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
methyl 4,6-dihydroxy-5-iodonicotinate		

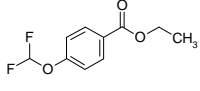
KD-0751	$C_8H_{10}N_2O_2S$	198.2451
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		0.0000
		rotatable bonds
		1.0000
		H-bond acceptors
		2.0000
H-bond donors		
2.0000		
LogP	-0.9439	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-amino-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxamide		

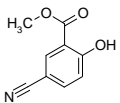
KD-0754	$C_9H_{11}NO_3S$	213.2569
		Halogen atoms
		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		3.0000
H-bond donors		
1.0000		
LogP	-0.0474	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
methyl 2-amino-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylate		

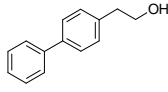
KD-0756	$C_7H_6ClF_3N_2$	210.5875
		Halogen atoms
		4.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		0.0000
H-bond donors		
2.0000		
LogP	1.8810	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
2-amino-4-chloro-5-(trifluoromethyl)phenylamine		

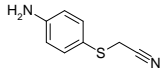
LC-0098	$C_6H_8N_2O_2$	140.1429
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		0.0000
		rotatable bonds
		0.0000
		H-bond acceptors
		2.0000
H-bond donors		
1.0000		
LogP	-0.5825	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
tetrahydro-1H-pyrrolo[1,2-c]imidazole-1,3(2H)-dione		

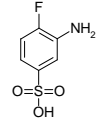
LC-0201	$C_{11}H_{10}O_3$	190.2006
		Halogen atoms
		0.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
0.0000		
LogP	1.8340	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
ethyl 1-benzofuran-2-carboxylate		

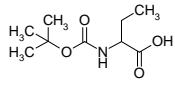
NC-0225	$C_{10}H_{10}F_2O_3$	216.1862
		Halogen atoms
		2.0000
		rotatable bonds
		5.0000
		H-bond acceptors
		3.0000
H-bond donors		
0.0000		
LogP	2.7207	
LogS	contact Key Organics for details	TPSA contact Key Organics for details
ethyl 4-(difluoromethoxy)benzenecarboxylate		

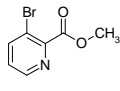
NC-0753	C ₉ H ₇ NO ₃	177.1610											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.3573</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	1.3573	
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.3573												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 5-cyano-2-hydroxybenzenecarboxylate													

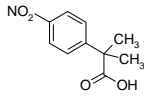
SS-2998	C ₁₄ H ₁₄ O	198.2671											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	3.4474												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[1,1'-biphenyl]-4-yl-1-ethanol													

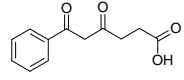
SS-2999	C ₈ H ₈ N ₂ S	164.2304											
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	1.0624												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[(4-aminophenyl)sulfanyl]acetonitrile													

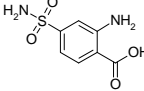
SS-3000	C ₆ H ₆ FNO ₃ S	191.1820											
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Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-amino-4-fluorobenzenesulfonic acid													

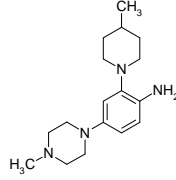
SS-3006	C ₉ H ₁₇ NO ₄	203.2401											
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[(tert-butoxycarbonyl)amino]butanoic acid													

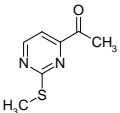
SS-3013	C ₇ H ₆ BrNO ₂	216.0354											
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H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 3-bromo-2-pyridinecarboxylate													

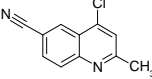
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rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	2.8586												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-methyl-2-(4-nitrophenyl)propanoic acid													

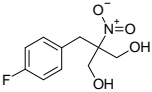
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Halogen atoms	0.0000												
rotatable bonds	6.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.5536												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4,6-dioxo-6-phenylhexanoic acid													

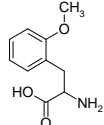
SS-3028	$C_7H_8N_2O_4S$	216.2168											
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H-bond acceptors	4.0000												
H-bond donors	3.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-amino-4-(aminosulfonyl)benzenecarboxylic acid													

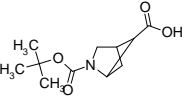
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rotatable bonds	2.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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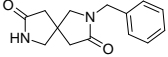
SS-3045	$C_7H_8N_2OS$	168.2186											
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rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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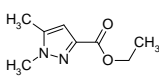
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Halogen atoms	1.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	3.1684												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-chloro-2-methyl-6-quinolinecarbonitrile													

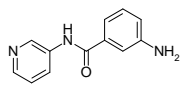
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Halogen atoms	1.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	1.3785												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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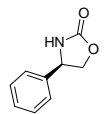
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.8996												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-amino-3-(2-methoxyphenyl)propanoic acid													

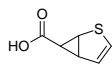
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rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	0.7073												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(tert-butoxycarbonyl)-2-azabicyclo[2.1.1]hexane-5-carboxylic acid													

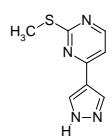
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	0.0961												
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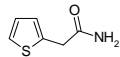
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 1,5-dimethyl-1H-pyrazole-3-carboxylate													


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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-amino-N-(3-pyridinyl)benzenecarboxamide													

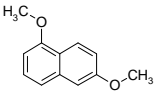
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(4R)-4-phenyl-1,3-oxazolan-2-one													

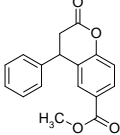
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
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LogP	0.3759												
													
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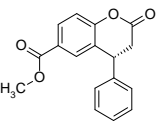
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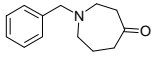
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	1.0000												
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LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
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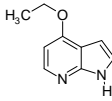
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Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	1.0000												
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LogP	0.1719												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-thiophenecarboxamide													

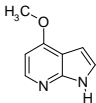
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Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	2.5434												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1,6-dimethoxynaphthalene													

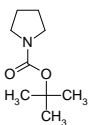
SS-3270	C ₁₇ H ₁₄ O ₄	282.2987	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	3.0184
		LogS	contact Key Organics for details
methyl 2-oxo-4-phenyl-6-chromanecarboxylate			

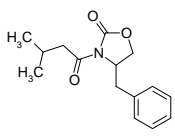
SS-3272	C ₁₇ H ₁₄ O ₄	282.2987	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	0.0000
		LogP	3.0184
		LogS	contact Key Organics for details
methyl (4R)-2-oxo-4-phenyl-3,4-dihydro-2H-chromene-6-carboxylate			

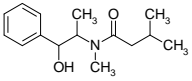
SS-3274	C ₁₃ H ₁₇ NO	203.2865	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	2.3465
		LogS	contact Key Organics for details
1-benzyl-4-azepanone			

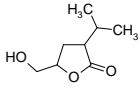
SS-3279	C ₉ H ₁₀ N ₂ O	162.1929	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	1.8207
		LogS	contact Key Organics for details
4-ethoxy-1H-pyrrolo[2,3-b]pyridine			

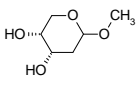
SS-3281	C ₈ H ₈ N ₂ O	148.1658	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	1.4782
		LogS	contact Key Organics for details
methyl 1H-pyrrolo[2,3-b]pyridin-4-yl ether			

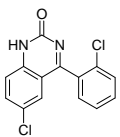
SS-3295	C ₉ H ₁₇ NO ₂	171.2413	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	1.2450
		LogS	contact Key Organics for details
tert-butyl 1-pyrrolidinecarboxylate			

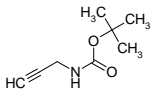
SS-3300	C ₁₅ H ₁₉ NO ₃	261.3236	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	3.1133
		LogS	contact Key Organics for details
4-benzyl-3-(3-methylbutanoyl)-1,3-oxazolan-2-one			

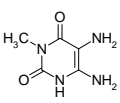
SS-3305	C ₁₅ H ₂₃ NO ₂	249.3561	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	2.6325
		LogS	contact Key Organics for details
N-(2-hydroxy-1-methyl-2-phenylethyl)-N,3-dimethylbutanamide			

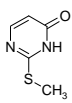
SS-3308	C ₈ H ₁₄ O ₃	158.1990	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.9232</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	0.9232
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.9232												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-(hydroxymethyl)-3-isopropylidihydro-2(3H)-furanone													

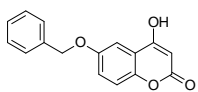
SS-3337	C ₆ H ₁₂ O ₄	148.1601	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>-0.4949</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	4.0000	H-bond donors	2.0000	LogP	-0.4949
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	-0.4949												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(3R,4S)-6-methoxytetrahydro-2H-pyran-3,4-diol													

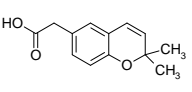
SS-3341	C ₁₄ H ₈ Cl ₂ N ₂ O	291.1387	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>4.0840</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	1.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	4.0840
Halogen atoms	2.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	4.0840												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-chloro-4-(2-chlorophenyl)-2(1H)-quinazolinone													

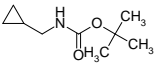
SS-3353	C ₈ H ₁₃ NO ₂	155.1983	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.9467</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	0.9467
Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	0.9467												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
tert-butyl N-(2-propynyl)carbamate													

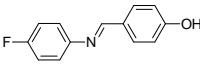
SS-3364	C ₅ H ₈ N ₄ O ₂	156.1451	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>3.0000</td></tr> <tr><td>LogP</td><td>-2.6795</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	0.0000	H-bond acceptors	2.0000	H-bond donors	3.0000	LogP	-2.6795
Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	3.0000												
LogP	-2.6795												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5,6-diamino-3-methyl-2,4(1H,3H)-pyrimidinedione													

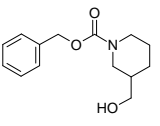
SS-3370	C ₅ H ₆ N ₂ OS	142.1804	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.5703</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	0.5703
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	0.5703												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(methylsulfanyl)-4(3H)-pyrimidinone													

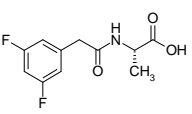
SS-3371	C ₁₆ H ₁₂ O ₄	268.2716	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.3187</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	2.3187
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	2.3187												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6-(benzyloxy)-4-hydroxy-2H-chromen-2-one													

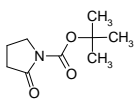
SS-3383	C ₁₃ H ₁₄ O ₃	218.2547	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.1785</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.1785
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.1785												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(2,2-dimethyl-2H-chromen-6-yl)acetic acid													

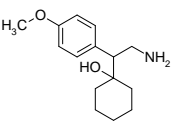
SS-3387	C ₉ H ₁₇ NO ₂	171.2413	
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			rotatable bonds
			4.0000
			H-bond acceptors
			2.0000
H-bond donors			
1.0000			
LogP	1.3828		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
tert-butyl N-(cyclopropylmethyl)carbamate			

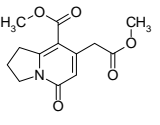
SS-3393	C ₁₃ H ₁₀ FNO	215.2292	
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			1.0000
			rotatable bonds
			3.0000
			H-bond acceptors
			2.0000
H-bond donors			
1.0000			
LogP	3.6769		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-((4-fluorophenyl)imino)methyl)benzenol			

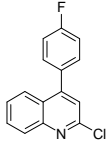
SS-3395	C ₁₄ H ₁₉ NO ₃	249.3124	
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			rotatable bonds
			4.0000
			H-bond acceptors
			3.0000
H-bond donors			
1.0000			
LogP	1.8846		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
benzyl 3-(hydroxymethyl)tetrahydro-1(2H)-pyridinecarboxylate			

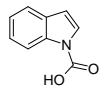
SS-3400	C ₁₁ H ₁₁ F ₂ NO ₃	243.2120	
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			2.0000
			rotatable bonds
			4.0000
			H-bond acceptors
			3.0000
H-bond donors			
2.0000			
LogP	1.4175		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
(2S)-2-([2-(3,5-difluorophenyl)acetyl]amino)propanoic acid			

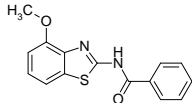
SS-3403	C ₉ H ₁₅ NO ₃	185.2248	
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			rotatable bonds
			2.0000
			H-bond acceptors
			3.0000
H-bond donors			
0.0000			
LogP	0.8137		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
tert-butyl 2-oxo-1-pyrrolidinecarboxylate			

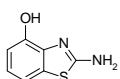
SS-3413	C ₁₅ H ₂₃ NO ₂	249.3561	
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			rotatable bonds
			4.0000
			H-bond acceptors
			3.0000
H-bond donors			
2.0000			
LogP	1.7841		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
1-[2-amino-1-(4-methoxyphenyl)ethyl]cyclohexanol			

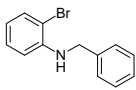
SS-3424	C ₁₃ H ₁₅ NO ₅	265.2682	
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			0.0000
			rotatable bonds
			5.0000
			H-bond acceptors
			5.0000
H-bond donors			
0.0000			
LogP	-1.4778		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
methyl 7-(2-methoxy-2-oxoethyl)-5-oxo-1,2,3,5-tetrahydro-8-indolizinecarboxylate			

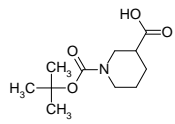
SS-3434	C ₁₅ H ₉ ClFN	257.6971	
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			2.0000
			rotatable bonds
			1.0000
			H-bond acceptors
			1.0000
H-bond donors			
0.0000			
LogP	4.8486		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
2-chloro-4-(4-fluorophenyl)quinoline			

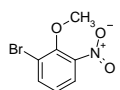
SS-3438	$C_9H_7NO_2$	161.1616											
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Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.4115												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1H-indole-1-carboxylic acid													

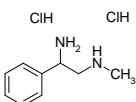
SS-3439	$C_{15}H_{12}N_2O_2S$	284.3391											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.8573												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-(4-methoxy-1,3-benzothiazol-2-yl)benzenecarboxamide													

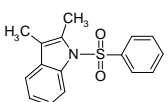
SS-3440	$C_7H_6N_2OS$	166.2027											
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Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	1.2806												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-amino-1,3-benzothiazol-4-ol													

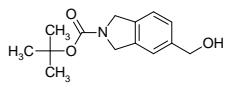
SS-3448	$C_{13}H_{12}BrN$	262.1513											
		<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>0.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>4.0456</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	0.0000	H-bond donors	1.0000	LogP	4.0456	
Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	0.0000												
H-bond donors	1.0000												
LogP	4.0456												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-benzyl-N-(2-bromophenyl)amine													

SS-3449	$C_{11}H_{19}NO_4$	229.2784											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.1157</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	1.1157	
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.1157												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(tert-butoxycarbonyl)-3-piperidinecarboxylic acid													

SS-3458	$C_7H_6BrNO_3$	232.0348											
		<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.5393</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	1.0000	H-bond acceptors	3.0000	H-bond donors	0.0000	LogP	2.5393	
Halogen atoms	1.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	0.0000												
LogP	2.5393												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-bromo-2-methoxy-3-nitrobenzene													

SS-3473	$C_9H_{16}Cl_2N_2$	223.1473											
		<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td></td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>1.4691</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds		H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	1.4691	
Halogen atoms	2.0000												
rotatable bonds													
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	1.4691												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(2-amino-2-phenylethyl)(methyl)amine dihydrochloride													

SS-3474	$C_{16}H_{15}NO_2S$	285.3675											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>3.8986</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	0.0000	LogP	3.8986	
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	3.8986												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2,3-dimethyl-1-(phenylsulfonyl)-1H-indole													

SS-3479	C ₁₄ H ₁₉ NO ₃	249.3124
		Halogen atoms 0.0000
		rotatable bonds 3.0000
		H-bond acceptors 3.0000
		H-bond donors 1.0000
		LogP 1.8907
LogS contact Key Organics for details	TPSA contact Key Organics for details	
tert-butyl 5-(hydroxymethyl)-1,3-dihydro-2H-isoindole-2-carboxylate		