



BIONET compounds –
A Key step ahead of the rest

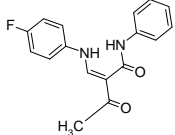
? arcZ 20#0

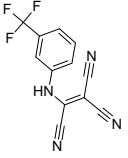
Fragments Collection Update

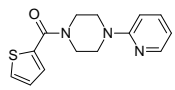


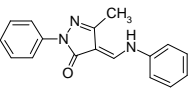
Key Organics

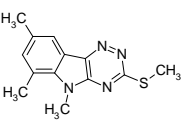
The right side of the Equation

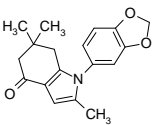
MS-7754	C ₁₇ H ₁₅ FN ₂ O ₂	298.3197	
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		rotatable bonds	6.0000
		H-bond acceptors	2.0000
		H-bond donors	2.0000
		LogP	1.8496
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
(Z)-2-acetyl-3-(4-fluoroanilino)-N-phenyl-2-propenamide			

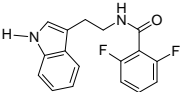
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		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.4303
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
2-[3-(trifluoromethyl)anilino]-1,1,2-ethylenetricarbonitrile			

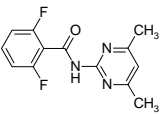
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		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	1.5346
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
[4-(2-pyridinyl)piperazino][2-thienyl)methanone			

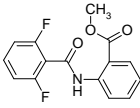
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		rotatable bonds	4.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	2.5336
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
4-[(E)-anilinomethylidene]-5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one			

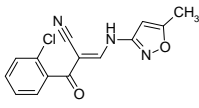
MS-7795	C ₁₃ H ₁₄ N ₄ S	258.3473	
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		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	3.1103
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
5,6,8-trimethyl-3-(methylsulfanyl)-5H-[1,2,4]triazino[5,6-b]indole			

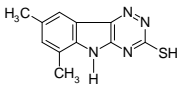
MS-7796	C ₁₈ H ₁₉ NO ₃	297.3570	
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		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	0.0000
		LogP	2.8461
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
1-(1,3-benzodioxol-5-yl)-2,6,6-trimethyl-1,5,6,7-tetrahydro-4H-indol-4-one			

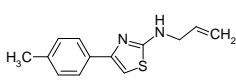
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		rotatable bonds	4.0000
		H-bond acceptors	1.0000
		H-bond donors	2.0000
		LogP	3.2072
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
2,6-difluoro-N-[2-(1H-indol-3-yl)ethyl]benzenecarboxamide			

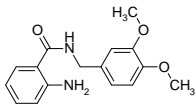
MS-7807	C ₁₃ H ₁₁ F ₂ N ₃ O	263.2489	
		Halogen atoms	2.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.9333
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-(4,6-dimethyl-2-pyrimidinyl)-2,6-difluorobenzenecarboxamide			

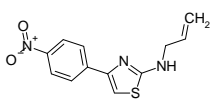
MS-7809	C ₁₅ H ₁₁ F ₂ NO ₃	291.2566	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.8175</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	4.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	2.8175
Halogen atoms	2.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.8175												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 2-((2,6-difluorobenzoyl)amino)benzenecarboxylate													

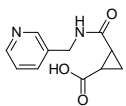
MS-7819	C ₁₄ H ₁₀ ClN ₃ O ₂	287.7077	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>5.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.4621</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	5.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	2.4621
Halogen atoms	1.0000												
rotatable bonds	5.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	2.4621												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
(E)-2-(2-chlorobenzoyl)-3-((5-methyl-3-isoxazolyl)amino)-2-propenenitrile													

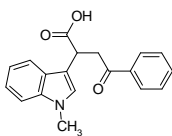
MS-7824	C ₁₁ H ₁₀ N ₄ S	230.2932	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>0.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>2.7296</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	0.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	2.7296
Halogen atoms	0.0000												
rotatable bonds	0.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	2.7296												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
6,8-dimethyl-5H-[1,2,4]triazino[5,6-b]indole-3-thiol													

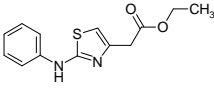
MS-7826	C ₁₃ H ₁₄ N ₂ S	230.3339	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>3.9046</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	3.9046
Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	3.9046												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-allyl-4-(4-methylphenyl)-1,3-thiazol-2-amine													

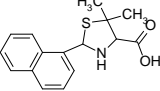
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	1.6147												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-amino-N-(3,4-dimethoxybenzyl)benzenecarboxamide													

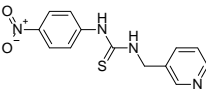
MS-7829	C ₁₂ H ₁₁ N ₃ O ₂ S	261.3044	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>3.3910</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	3.3910
Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	3.3910												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-allyl-4-(4-nitrophenyl)-1,3-thiazol-2-amine													

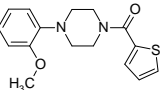
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.1598												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-((3-pyridinylmethyl)amino)carbonylcyclopropanecarboxylic acid													

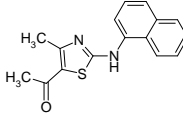
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	2.9463												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(1-methyl-1H-indol-3-yl)-4-oxo-4-phenylbutanoic acid													

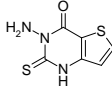
MS-7837	C ₁₃ H ₁₄ N ₂ O ₂ S	262.3327	
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		rotatable bonds	6.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.6992
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 2-(2-anilino-1,3-thiazol-4-yl)acetate			

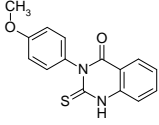
MS-7838	C ₁₆ H ₁₇ NO ₂ S	287.3834	
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		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	3.2398
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
5,5-dimethyl-2-(1-naphthyl)-1,3-thiazolane-4-carboxylic acid			

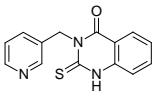
MS-7849	C ₁₃ H ₁₂ N ₄ O ₂ S	288.3302	
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		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	3.1548
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
N-(4-nitrophenyl)-N'-(3-pyridinylmethyl)thiourea			

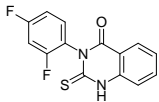
MS-7856	C ₁₆ H ₁₈ N ₂ O ₂ S	302.3981	
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		rotatable bonds	3.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	1.8952
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
[4-(2-methoxyphenyl)piperazino][2-thienyl]methanone			

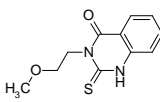
MS-7863	C ₁₆ H ₁₄ N ₂ OS	282.3668	
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		rotatable bonds	3.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	3.0193
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
1-[4-methyl-2-(1-naphthylamino)-1,3-thiazol-5-yl]-1-ethanone			

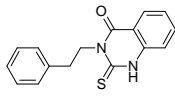
MS-7867	C ₆ H ₅ N ₃ OS ₂	199.2543	
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		rotatable bonds	0.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	0.8351
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-amino-2-thioxo-2,3-dihydrothieno[3,2-d]pyrimidin-4(1H)-one			

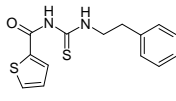
MS-7886	C ₁₅ H ₁₂ N ₂ O ₂ S	284.3391	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	3.2317
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-(4-methoxyphenyl)-2-thioxo-2,3-dihydro-4(1H)-quinazolinone			

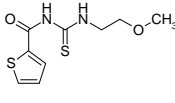
MS-7888	C ₁₄ H ₁₁ N ₃ OS	269.3273	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	2.7323
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-(3-pyridinylmethyl)-2-thioxo-2,3-dihydro-4(1H)-quinazolinone			

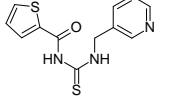
MS-7890	C ₁₄ H ₈ F ₂ N ₂ OS	290.2935
	Halogen atoms	2.0000
	rotatable bonds	1.0000
	H-bond acceptors	2.0000
	H-bond donors	1.0000
	LogP	3.7634
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
3-(2,4-difluorophenyl)-2-thioxo-2,3-dihydro-4(1H)-quinazolinone		

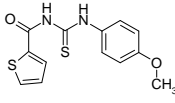
MS-7891	C ₁₁ H ₁₂ N ₂ O ₂ S	236.2945
	Halogen atoms	0.0000
	rotatable bonds	3.0000
	H-bond acceptors	3.0000
	H-bond donors	1.0000
	LogP	1.6379
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
3-(2-methoxyethyl)-2-thioxo-2,3-dihydro-4(1H)-quinazolinone		

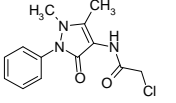
MS-7892	C ₁₆ H ₁₄ N ₂ OS	282.3668
	Halogen atoms	0.0000
	rotatable bonds	3.0000
	H-bond acceptors	2.0000
	H-bond donors	1.0000
	LogP	3.8310
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
3-phenethyl-2-thioxo-2,3-dihydro-4(1H)-quinazolinone		

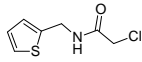
MS-7893	C ₁₄ H ₁₄ N ₂ O ₂ S ₂	290.4085
	Halogen atoms	0.0000
	rotatable bonds	6.0000
	H-bond acceptors	2.0000
	H-bond donors	2.0000
	LogP	3.2411
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
N-phenethyl-N'-(2-thienylcarbonyl)thiourea		

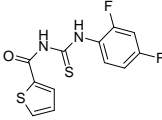
MS-7894	C ₉ H ₁₂ N ₂ O ₂ S ₂	244.3362
	Halogen atoms	0.0000
	rotatable bonds	6.0000
	H-bond acceptors	3.0000
	H-bond donors	2.0000
	LogP	1.0480
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
N-(2-methoxyethyl)-N'-(2-thienylcarbonyl)thiourea		

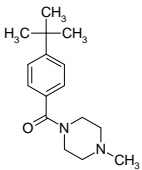
MS-7895	C ₁₂ H ₁₁ N ₃ O ₂ S ₂	277.3690
	Halogen atoms	0.0000
	rotatable bonds	5.0000
	H-bond acceptors	3.0000
	H-bond donors	2.0000
	LogP	2.1424
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
N-(3-pyridinylmethyl)-N'-(2-thienylcarbonyl)thiourea		

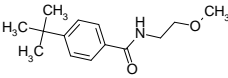
MS-7897	C ₁₃ H ₁₂ N ₂ O ₂ S ₂	292.3808
	Halogen atoms	0.0000
	rotatable bonds	5.0000
	H-bond acceptors	3.0000
	H-bond donors	2.0000
	LogP	2.6418
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
N-(4-methoxyphenyl)-N'-(2-thienylcarbonyl)thiourea		

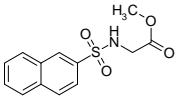
MS-7905	C ₁₃ H ₁₄ ClN ₃ O ₂	279.7284
	Halogen atoms	1.0000
	rotatable bonds	3.0000
	H-bond acceptors	2.0000
	H-bond donors	1.0000
	LogP	
	TPSA	
LogS	contact Key Organics for details	contact Key Organics for details
2-chloro-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)acetamide		

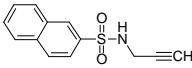
MS-7907	C ₇ H ₈ CINOS	189.6649	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.8732</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	0.8732
Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	0.8732												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-chloro-N-(2-thienylmethyl)acetamide													

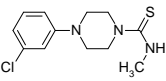
MS-7913	C ₁₂ H ₈ F ₂ N ₂ OS ₂	298.3352	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>3.1735</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	4.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	3.1735
Halogen atoms	2.0000												
rotatable bonds	4.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	3.1735												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-(2,4-difluorophenyl)-N'-(2-thienylcarbonyl)thiourea													

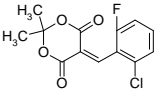
MS-7921	C ₁₆ H ₂₄ N ₂ O	260.3825	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>2.8017</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	0.0000	LogP	2.8017
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	0.0000												
LogP	2.8017												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
[4-(tert-butyl)phenyl][4-methylpiperazino]methanone													

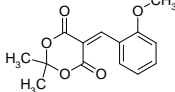
MS-7922	C ₁₄ H ₂₁ NO ₂	235.3290	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>5.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.5891</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	5.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	2.5891
Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.5891												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(tert-butyl)-N-(2-methoxyethyl)benzenecarboxamide													

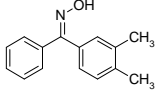
MS-7929	C ₁₃ H ₁₃ NO ₄ S	279.3169	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>5.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.3885</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	5.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	1.3885
Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.3885												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
methyl 2-[(2-naphthylsulfonyl)amino]acetate													

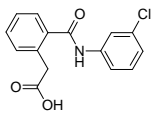
MS-7931	C ₁₃ H ₁₁ NO ₂ S	245.3021	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>4.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.0888</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	4.0000	H-bond acceptors	2.0000	H-bond donors	1.0000	LogP	2.0888
Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	2.0888												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-(2-propynyl)-2-naphthalenesulfonamide													

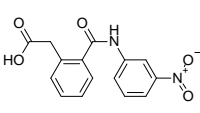
MS-7938	C ₁₂ H ₁₆ ClN ₃ S	269.7984	<table border="1"> <tr><td>Halogen atoms</td><td>1.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>1.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>2.9523</td></tr> </table>	Halogen atoms	1.0000	rotatable bonds	3.0000	H-bond acceptors	1.0000	H-bond donors	1.0000	LogP	2.9523
Halogen atoms	1.0000												
rotatable bonds	3.0000												
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.9523												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(3-chlorophenyl)-N-methyltetrahydro-1(2H)-pyrazinecarbothioamide													

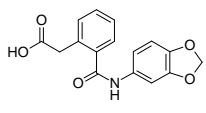
MS-7952	C ₁₃ H ₁₀ ClFO ₄	284.6737	<table border="1"> <tr><td>Halogen atoms</td><td>2.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>0.0000</td></tr> <tr><td>LogP</td><td>3.2070</td></tr> </table>	Halogen atoms	2.0000	rotatable bonds	2.0000	H-bond acceptors	4.0000	H-bond donors	0.0000	LogP	3.2070
Halogen atoms	2.0000												
rotatable bonds	2.0000												
H-bond acceptors	4.0000												
H-bond donors	0.0000												
LogP	3.2070												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
5-[(2-chloro-6-fluorophenyl)methylene]-2,2-dimethyl-1,3-dioxane-4,6-dione													

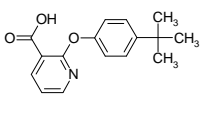
MS-7953	C ₁₄ H ₁₄ O ₅	262.2647	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	5.0000
		H-bond donors	0.0000
		LogP	2.2968
		LogS	contact Key Organics for details
5-[(2-methoxyphenyl)methylene]-2,2-dimethyl-1,3-dioxane-4,6-dione			

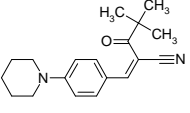
MS-7954	C ₁₅ H ₁₅ NO	225.2929	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	4.8599
		LogS	contact Key Organics for details
(3,4-dimethylphenyl)(phenyl)methanone oxime			

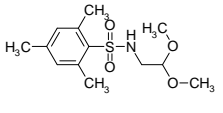
MS-7957	C ₁₅ H ₁₂ ClNO ₃	289.7208	
		Halogen atoms	1.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	2.9573
		LogS	contact Key Organics for details
2-{2-[(3-chloroanilino)carbonyl]phenyl}acetic acid			

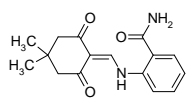
MS-7959	C ₁₅ H ₁₂ N ₂ O ₅	300.2733	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	5.0000
		H-bond donors	2.0000
		LogP	2.3929
		LogS	contact Key Organics for details
2-{2-[(3-nitroanilino)carbonyl]phenyl}acetic acid			

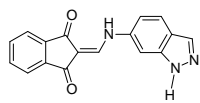
MS-7962	C ₁₆ H ₁₃ NO ₅	299.2857	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	5.0000
		H-bond donors	2.0000
		LogP	1.7738
		LogS	contact Key Organics for details
2-{2-[(1,3-benzodioxol-5-ylamino)carbonyl]phenyl}acetic acid			

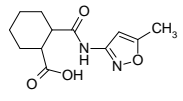
MS-7971	C ₁₆ H ₁₇ NO ₃	271.3188	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	4.6528
		LogS	contact Key Organics for details
2-[4-(tert-butyl)phenoxy]nicotinic acid			

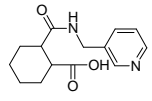
MS-7975	C ₁₉ H ₂₄ N ₂ O	296.4159	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	2.0000
		H-bond donors	0.0000
		LogP	3.8083
		LogS	contact Key Organics for details
(Z)-2-(2,2-dimethylpropanoyl)-3-(4-piperidinophenyl)-2-propenenitrile			

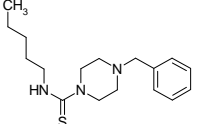
MS-7994	C ₁₃ H ₂₁ NO ₄ S	287.3806	
		Halogen atoms	0.0000
		rotatable bonds	6.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	2.2224
		LogS	contact Key Organics for details
N-(2,2-dimethoxyethyl)-2,4,6-trimethylbenzenesulfonamide			

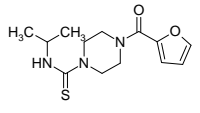
MS-8003	C ₁₆ H ₁₈ N ₂ O ₃	286.3335	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	0.2102
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
2-[[[4,4-dimethyl-2,6-dioxocyclohexylidene)methyl]amino]benzenecarboxamide			

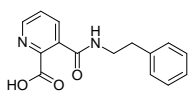
MS-8004	C ₁₇ H ₁₁ N ₃ O ₂	289.2961	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	1.1298
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
2-[(1H-indazol-6-ylamino)methylene]-1H-indene-1,3(2H)-dione			

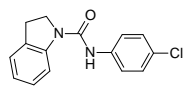
MS-8011	C ₁₂ H ₁₆ N ₂ O ₄	252.2723	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	5.0000
		H-bond donors	2.0000
		LogP	1.3187
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
2-[[[5-methyl-3-isoxazolyl)amino]carbonyl]cyclohexanecarboxylic acid			

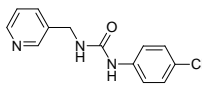
MS-8013	C ₁₄ H ₁₈ N ₂ O ₃	262.3112	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	1.3487
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
2-[[[3-pyridinyl)methyl]amino]carbonyl]cyclohexanecarboxylic acid			

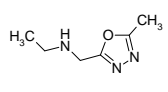
MS-8017	C ₁₇ H ₂₇ N ₃ S	305.4888	
		Halogen atoms	0.0000
		rotatable bonds	8.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	4.1329
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
4-benzyl-N-pentyltetrahydro-1(2H)-pyrazinecarbothioamide			

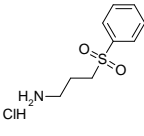
MS-8018	C ₁₃ H ₁₉ N ₃ O ₂ S	281.3793	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.6729
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
4-(2-furylcarbonyl)-N-isopropyltetrahydro-1(2H)-pyrazinecarbothioamide			

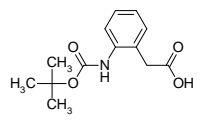
MS-8021	C ₁₅ H ₁₄ N ₂ O ₃	270.2904	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	2.4055
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
3-[(phenethylamino)carbonyl]-2-pyridinecarboxylic acid			

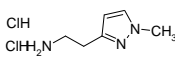
MS-8025	C ₁₅ H ₁₃ ClN ₂ O	272.7367	
		Halogen atoms	1.0000
		rotatable bonds	1.0000
		H-bond acceptors	1.0000
		H-bond donors	1.0000
		LogP	3.1238
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-(4-chlorophenyl)-1-indolinecarboxamide			


MS-8026	C ₁₃ H ₁₂ ClN ₃ O	261.7131	
		Halogen atoms	1.0000
		rotatable bonds	3.0000
		H-bond acceptors	2.0000
		H-bond donors	2.0000
		LogP	2.3184
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
N-(4-chlorophenyl)-N'-(3-pyridinylmethyl)urea			

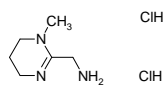
SS-3821	C ₆ H ₁₁ N ₃ O	141.1741	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	0.3307
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
N-[(5-methyl-1,3,4-oxadiazol-2-yl)methyl]ethanamine			

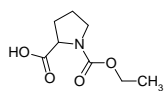
SS-3822	C ₉ H ₁₄ ClNO ₂ S	235.7344	
		Halogen atoms	1.0000
		rotatable bonds	
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.7616
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-benzenesulfonylpropylamine hydrochloride			

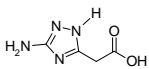
SS-3824	C ₁₃ H ₁₇ NO ₄	251.2847	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	1.9855
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
BOC-(aminophenyl)acetic acid			

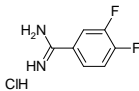
SS-3827	C ₆ H ₁₃ Cl ₂ N ₃	198.0966	
		Halogen atoms	2.0000
		rotatable bonds	
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	0.8059
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-aminoethyl-1-methylpyrazole dihydrochloride			

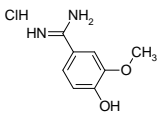
SS-3828	C ₄ H ₈ Cl ₂ N ₂ S	187.0918	
		Halogen atoms	2.0000
		rotatable bonds	
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	0.2365
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
Thiazol-5-yl-methylamine dihydrochloride			

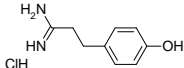
SS-3831	C ₆ H ₁₅ Cl ₂ N ₃	200.1126	
		Halogen atoms	2.0000
		rotatable bonds	
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	-0.0853
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
(1-methyl-1,4,5,6 tetrahydro-pyrimidin-2-yl)-methylamine dihydrochloride			

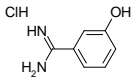
SS-3834	C ₈ H ₁₃ NO ₄	187.1971	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	0.4905
		TPSA	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
pyrrolidine-1,2-dicarboxylic acid 1-ethyl ester			

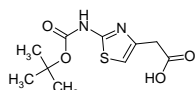
SS-3835	$C_4H_6N_4O_2$	142.1180	
			
		Halogen atoms 0.0000	
		rotatable bonds 2.0000	
		H-bond acceptors 4.0000	
		H-bond donors 3.0000	
		LogP -0.3970	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
(3-amino-1H-1,2,4-triazol-5-yl)acetic acid			

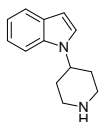
SS-3844	$C_7H_7ClF_2N_2$	192.5970	
			
		Halogen atoms 3.0000	
		rotatable bonds	
		H-bond acceptors 1.0000	
		H-bond donors 1.0000	
		LogP 1.8107	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3,4-difluoro-benzamidine hydrochloride			

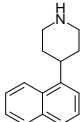
SS-3845	$C_8H_{11}ClN_2O_2$	202.6421	
			
		Halogen atoms 1.0000	
		rotatable bonds	
		H-bond acceptors 3.0000	
		H-bond donors 2.0000	
		LogP 0.9946	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-hydroxy-3-methoxybenzamide hydrochloride			

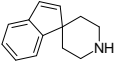
SS-3846	$C_9H_{13}ClN_2O$	200.6698	
			
		Halogen atoms 1.0000	
		rotatable bonds	
		H-bond acceptors 2.0000	
		H-bond donors 2.0000	
		LogP 1.5761	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-(4-hydroxy-phenyl)-propionamide hydrochloride			

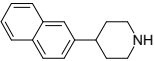
SS-3847	$C_7H_9ClN_2O$	172.6156	
			
		Halogen atoms 1.0000	
		rotatable bonds	
		H-bond acceptors 2.0000	
		H-bond donors 2.0000	
		LogP 1.2473	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
3-hydroxybenzamide hydrochloride			

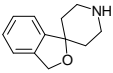
SS-3851	$C_{10}H_{14}N_2O_4S$	258.2981	
			
		Halogen atoms 0.0000	
		rotatable bonds 5.0000	
		H-bond acceptors 5.0000	
		H-bond donors 2.0000	
		LogP 1.5207	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
N-BOC-2-amino-4-thiazolacetic acid			

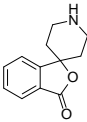
SS-3855	$C_{13}H_{17}ClN_2$	236.7468	
			
		Halogen atoms 1.0000	
		rotatable bonds	
		H-bond acceptors 1.0000	
		H-bond donors 1.0000	
		LogP 1.9895	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-(1-indole)piperidine hydrochloride			

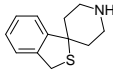
SS-3856	$C_{15}H_{18}ClN$	247.7704	
			
		Halogen atoms 1.0000	
		rotatable bonds	
		H-bond acceptors 1.0000	
		H-bond donors 1.0000	
		LogP 3.3758	
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-(1-naphthyl)piperidine hydrochloride			

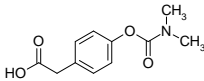
SS-3857	C ₁₃ H ₁₆ ClN	221.7322	
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			rotatable bonds
			0
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	2.5098		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-spiroindene-piperidine hydrochloride			

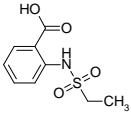
SS-3858	C ₁₅ H ₁₈ ClN	247.7704	
			Halogen atoms
			1.0000
			rotatable bonds
			0
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	3.3758		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-(2-naphthyl)piperidine hydrochloride			

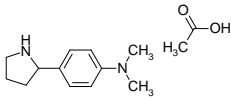
SS-3860	C ₁₂ H ₁₆ ClNO	225.7204	
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			rotatable bonds
			0
			H-bond acceptors
2.0000			
H-bond donors			
1.0000			
LogP	1.1785		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-spiro[1-phthalan]piperidine hydrochloride			

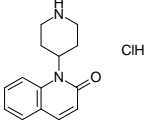
SS-3861	C ₁₂ H ₁₄ ClNO ₂	239.7039	
			Halogen atoms
			1.0000
			rotatable bonds
			0
			H-bond acceptors
3.0000			
H-bond donors			
1.0000			
LogP	1.1656		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-Spiro[3-phthalide]piperidine hydrochloride			

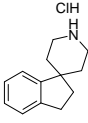
SS-3862	C ₁₂ H ₁₆ ClNS	241.7850	
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			1.0000
			rotatable bonds
			0
			H-bond acceptors
1.0000			
H-bond donors			
1.0000			
LogP	1.6210		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-Spiro[1-thiophthalane] piperidine hydrochloride			

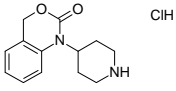
SS-3863	C ₁₁ H ₁₃ NO ₄	223.2306	
			Halogen atoms
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			rotatable bonds
			4.0000
			H-bond acceptors
4.0000			
H-bond donors			
1.0000			
LogP	1.3982		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
4-(dimethylcarbamoyloxy)phenylacetic acid			

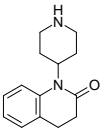
SS-3864	C ₉ H ₁₁ NO ₄ S	229.2563	
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			rotatable bonds
			4.0000
			H-bond acceptors
4.0000			
H-bond donors			
2.0000			
LogP	0.8537		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
2-(Ethanesulphonylamino)benzoic acid			

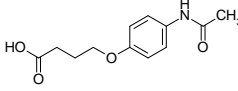
SS-3871	C ₁₄ H ₂₂ N ₂ O ₂	250.3436	
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			rotatable bonds
			2.0000
			H-bond acceptors
3.0000			
H-bond donors			
2.0000			
LogP	1.5924		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
dimethyl-(4-pyrrolidin-2-yl-phenyl)-amine monoacetate			

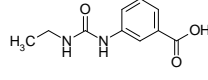
SS-3872	C ₁₄ H ₁₇ ClN ₂ O	264.7574											
													
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.3395												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(4-piperidyl)-1,2-dihydro-2-quinolinone													

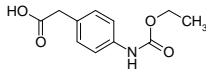
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	1.0000												
H-bond donors	1.0000												
LogP	2.7700												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-Spiroindane-piperidine hydrochloride													

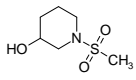
SS-3874	C ₁₃ H ₁₇ ClN ₂ O ₂	268.7456											
													
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.4205												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(piperidin-4-yl)-1H-benzodioxazine-2(4H)-one hydrochloride													

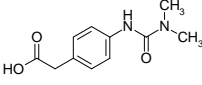
SS-3875	C ₁₄ H ₁₉ ClN ₂ O	266.7733											
													
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	2.0000												
H-bond donors	1.0000												
LogP	1.2603												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(4-piperidyl)-1,2,3,4-tetrahydro-2-quinolinone hydrochloride													

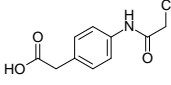
SS-3876	C ₁₂ H ₁₅ NO ₄	237.2577											
													
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Halogen atoms	0.0000												
rotatable bonds	6.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.6176												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-[4-(acetylamino)phenoxy]butanoic acid													

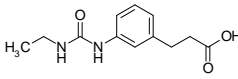
SS-3880	C ₁₀ H ₁₂ N ₂ O ₃	208.2187											
													
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	3.0000												
LogP	0.9117												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-[(ethylamino)carbonyl]aminobenzoic acid													

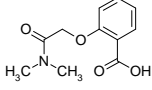
SS-3881	C ₁₁ H ₁₃ NO ₄	223.2306											
													
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	1.4942												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-[4-[(ethoxycarbonyl)amino]phenyl]acetic acid													

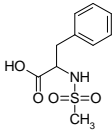
SS-3883	C ₆ H ₁₃ NO ₃ S	179.2394											
													
			<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>1.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>-0.6693</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	1.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	-0.6693
Halogen atoms	0.0000												
rotatable bonds	1.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	-0.6693												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(methylsulfonyl)-3-piperidinol													

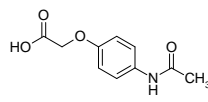
SS-3888	$C_{11}H_{14}N_2O_3$	222.2458
		Halogen atoms
		0.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		3.0000
H-bond donors		
2.0000		
LogP	0.7482	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
2-(4-((dimethylamino)carbonyl)amino)phenyl)acetic acid		

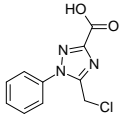
SS-3889	$C_{10}H_{10}ClNO_3$	227.6491
		Halogen atoms
		1.0000
		rotatable bonds
		4.0000
		H-bond acceptors
		3.0000
H-bond donors		
2.0000		
LogP	1.1175	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
(4-((chloroacetyl)amino)phenyl)acetic acid		

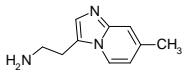
SS-3890	$C_{12}H_{16}N_2O_3$	236.2729
		Halogen atoms
		0.0000
		rotatable bonds
		5.0000
		H-bond acceptors
		3.0000
H-bond donors		
3.0000		
LogP	1.2405	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
3-(3-((ethylamino)carbonyl)aminophenyl)propanoic acid		

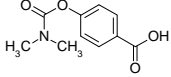
SS-3894	$C_{11}H_{13}NO_4$	223.2306
		Halogen atoms
		0.0000
		rotatable bonds
		4.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	0.6623	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
2-((dimethylcarbamoyl)methoxy)benzoic acid		

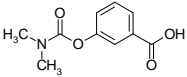
SS-3895	$C_{10}H_{13}NO_4S$	243.2834
		Halogen atoms
		0.0000
		rotatable bonds
		5.0000
		H-bond acceptors
		4.0000
H-bond donors		
2.0000		
LogP	0.8962	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
N-(methylsulfonyl)-DL-phenylalanine		

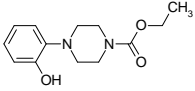
SS-3896	$C_{10}H_{11}NO_4$	209.2035
		Halogen atoms
		0.0000
		rotatable bonds
		4.0000
		H-bond acceptors
		4.0000
H-bond donors		
2.0000		
LogP	0.1846	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
(4-acetamidophenoxy)acetic acid		

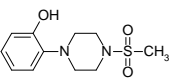
SS-3900	$C_{10}H_8ClN_3O_2$	237.6472
		Halogen atoms
		1.0000
		rotatable bonds
		3.0000
		H-bond acceptors
		4.0000
H-bond donors		
1.0000		
LogP	2.9201	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
5-(chloromethyl)-1-phenyl-1H-1,2,4-triazole-3-carboxylic acid		

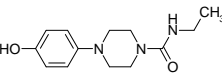
SS-3901	$C_{10}H_{13}N_3$	175.2352
		Halogen atoms
		0.0000
		rotatable bonds
		2.0000
		H-bond acceptors
		2.0000
H-bond donors		
1.0000		
LogP	0.7087	
LogS	contact Key Organics for details	TPSA
contact Key Organics for details		contact Key Organics for details
3-(2-aminoethyl)-7-methyl-imidazo[1,2-a]pyridine		

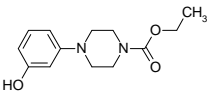
SS-3903	$C_{10}H_{11}NO_4$	209.2035	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.4657</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	1.4657
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.4657												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-N,N-dimethylcarbamoyloxy-benzoic acid													

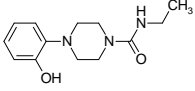
SS-3904	$C_{10}H_{11}NO_4$	209.2035	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>4.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.4657</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	4.0000	H-bond donors	1.0000	LogP	1.4657
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	1.4657												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-dimethylcarbamoyloxy-benzoic acid													

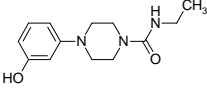
SS-3906	$C_{13}H_{18}N_2O_3$	250.3000	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.6267</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.6267
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.6267												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(2-hydroxyphenyl)-4-ethoxycarbonyl-piperazine													

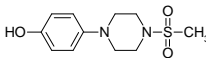
SS-3907	$C_{11}H_{16}N_2O_3S$	256.3258	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>0.5762</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	0.5762
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.5762												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(2-hydroxyphenyl)piperazin-4-methylsulfonamide													

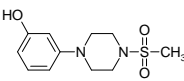
SS-3908	$C_{13}H_{19}N_3O_2$	249.3153	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.9767</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	0.9767
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.9767												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(4-hydroxyphenyl)-4-ethylcarbamoyl-piperazine													

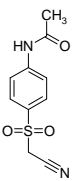
SS-3909	$C_{13}H_{18}N_2O_3$	250.3000	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>1.0000</td></tr> <tr><td>LogP</td><td>1.6267</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	1.0000	LogP	1.6267
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.6267												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(3-hydroxyphenyl)-4-ethoxycarbonyl-piperazine													

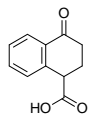
SS-3910	$C_{13}H_{19}N_3O_2$	249.3153	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.9767</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	0.9767
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.9767												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(2-hydroxyphenyl)-4-ethylcarbamoyl-piperazine													

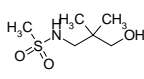
SS-3911	$C_{13}H_{19}N_3O_2$	249.3153	<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>2.0000</td></tr> <tr><td>H-bond acceptors</td><td>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.9767</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	2.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	0.9767
Halogen atoms	0.0000												
rotatable bonds	2.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.9767												
													
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(3-hydroxyphenyl)-4-ethylcarbamoyl-piperazine													

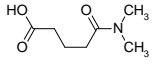
SS-3912	C ₁₁ H ₁₆ N ₂ O ₃ S	256.3258	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.5762
		LogS	contact Key Organics for details
4-(4-(methylsulfonyl)piperazin-1-yl)phenol			

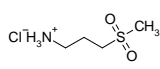
SS-3913	C ₁₁ H ₁₆ N ₂ O ₃ S	256.3258	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	0.5762
		LogS	contact Key Organics for details
3-(4-(methylsulfonyl)piperazin-1-yl)phenol			

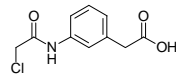
SS-3915	C ₁₀ H ₁₀ N ₂ O ₃ S	238.2668	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	-0.2511
		LogS	contact Key Organics for details
4-(acetamidophenylsulfonyl)acetonitrile			

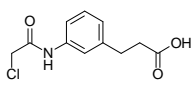
SS-3938	C ₁₁ H ₁₀ O ₃	190.2006	
		Halogen atoms	0.0000
		rotatable bonds	1.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.2763
		LogS	contact Key Organics for details
4-oxo-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid			

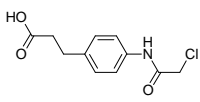
SS-3940	C ₆ H ₁₅ NO ₃ S	181.2553	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	-0.1520
		LogS	contact Key Organics for details
N-(3-hydroxy-2,2-dimethylpropyl)methanesulfonamide			

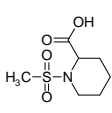
SS-3941	C ₇ H ₁₃ NO ₃	159.1866	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	-0.3515
		LogS	contact Key Organics for details
5-(dimethylamino)-5-oxopentanoic acid			

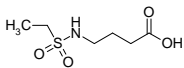
SS-3945	C ₄ H ₁₂ ClNO ₂ S	173.6627	
		Halogen atoms	1.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	1.0000
		LogP	1.0000
		LogS	contact Key Organics for details
3-methanesulfonyl-propyl-ammonium; chloride			

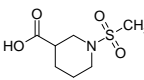
SS-3946	C ₁₀ H ₁₀ ClNO ₃	227.6491	
		Halogen atoms	1.0000
		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	1.1175
		LogS	contact Key Organics for details
N-Chloroacetyl-3-aminophenylacetic acid			

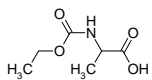
SS-3947	C ₁₁ H ₁₂ ClNO ₃	241.6762	
		Halogen atoms	1.0000
		rotatable bonds	5.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	1.5138
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-chloroacetyl-3-aminophenylpropionic acid			

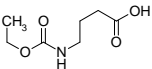
SS-3948	C ₁₁ H ₁₂ ClNO ₃	241.6762	
		Halogen atoms	1.0000
		rotatable bonds	5.0000
		H-bond acceptors	3.0000
		H-bond donors	2.0000
		LogP	1.5138
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-chloroacetyl-4-aminophenylpropionic acid			

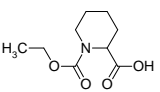
SS-3952	C ₇ H ₁₃ NO ₄ S	207.2500	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	-0.1637
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
1-(methylsulfonyl)piperidine-2-carboxylic acid			

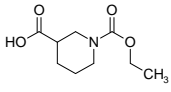
SS-3953	C ₆ H ₁₃ NO ₄ S	195.2388	
		Halogen atoms	0.0000
		rotatable bonds	6.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	-0.5516
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-(ethylsulfonyl)-4-aminobutyric acid			

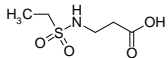
SS-3954	C ₇ H ₁₃ NO ₄ S	207.2500	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	-0.4261
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
1-(methylsulfonyl)piperidine-3-carboxylic acid			

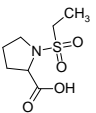
SS-3955	C ₆ H ₁₁ NO ₄	161.1589	
		Halogen atoms	0.0000
		rotatable bonds	4.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	0.2609
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-(ethoxycarbonyl)-DL-alanine			

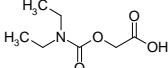
SS-3956	C ₇ H ₁₃ NO ₄	175.1860	
		Halogen atoms	0.0000
		rotatable bonds	6.0000
		H-bond acceptors	4.0000
		H-bond donors	2.0000
		LogP	0.1564
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
N-(ethoxycarbonyl)-4-aminobutyric acid			

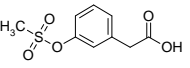
SS-3957	C ₉ H ₁₅ NO ₄	201.2242	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	4.0000
		H-bond donors	1.0000
		LogP	0.8868
		LogS	TPSA
contact Key Organics for details		contact Key Organics for details	
1-(ethoxycarbonyl)piperidine-2-carboxylic acid			

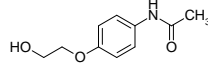
SS-3958	C ₉ H ₁₅ NO ₄	201.2242		Halogen atoms 0.0000 rotatable bonds 3.0000 H-bond acceptors 4.0000 H-bond donors 1.0000 LogP 0.6244
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
1-(ethoxycarbonyl)piperidine-3-carboxylic acid				

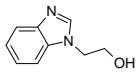
SS-3961	C ₅ H ₁₁ NO ₄ S	181.2117		Halogen atoms 0.0000 rotatable bonds 5.0000 H-bond acceptors 4.0000 H-bond donors 2.0000 LogP -0.8033
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
N-(ethylsulfonyl)-beta-alanine				

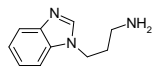
SS-3962	C ₇ H ₁₃ NO ₄ S	207.2500		Halogen atoms 0.0000 rotatable bonds 3.0000 H-bond acceptors 4.0000 H-bond donors 1.0000 LogP -0.2175
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
N-(ethylsulfonyl)-DL-proline				

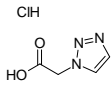
SS-3963	C ₇ H ₁₃ NO ₄	175.1860		Halogen atoms 0.0000 rotatable bonds 5.0000 H-bond acceptors 4.0000 H-bond donors 1.0000 LogP 0.3124
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
2-(diethylcarbamoyl)acetic acid				

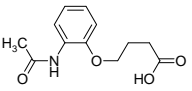
SS-3964	C ₉ H ₁₀ O ₅ S	230.2411		Halogen atoms 0.0000 rotatable bonds 4.0000 H-bond acceptors 5.0000 H-bond donors 1.0000 LogP
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
3-[(methylsulfonyl)oxy]phenylacetic acid				

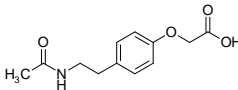
SS-3965	C ₁₀ H ₁₃ NO ₃	195.2200		Halogen atoms 0.0000 rotatable bonds 4.0000 H-bond acceptors 3.0000 H-bond donors 2.0000 LogP 0.1997
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
N-[4-(hydroxyethoxy)phenyl]ethanamide				

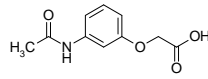
SS-3966	C ₉ H ₁₀ N ₂ O	162.1929		Halogen atoms 0.0000 rotatable bonds 2.0000 H-bond acceptors 2.0000 H-bond donors 1.0000 LogP 0.7214
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
1-(2-hydroxyethyl)benzimidazole				

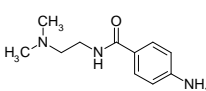
SS-3967	C ₁₀ H ₁₃ N ₃	175.2352		Halogen atoms 0.0000 rotatable bonds 3.0000 H-bond acceptors 2.0000 H-bond donors 1.0000 LogP 0.4260
LogS	contact Key Organics for details	TPSA	contact Key Organics for details	
3-(1H-benzimidazol-1-yl)propylamine				

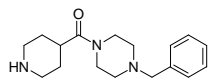
SS-3969	C ₄ H ₆ ClN ₃ O ₂	163.5643											
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	4.0000												
H-bond donors	1.0000												
LogP	0.4840												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1H-1,2,3 Triazole-1- acetic acid Hydrochloride													

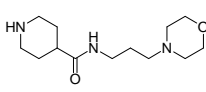
SS-3970	C ₁₂ H ₁₅ NO ₄	237.2577											
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Halogen atoms	0.0000												
rotatable bonds	6.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.6176												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(2-acetamidophenoxy)butanoic acid													

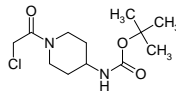
SS-3971	C ₁₂ H ₁₅ NO ₄	237.2577											
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Halogen atoms	0.0000												
rotatable bonds	6.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.5312												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(2-acetamidoethyl)phenoxyacetic acid													

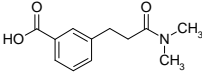
SS-3972	C ₁₀ H ₁₁ NO ₄	209.2035											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	0.1846												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
3-acetamidophenoxyacetic acid													

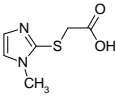
SS-3976	C ₁₁ H ₁₇ N ₃ O	207.2776											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.3226												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-amino-N-[2-(dimethylamino)ethyl]benzamide													

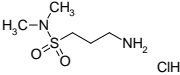
SS-3977	C ₁₇ H ₂₅ N ₃ O	287.4083											
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Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.0533												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-benzyl-4-(piperidin-4-ylcarbonyl)piperazine													

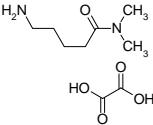
SS-3979	C ₁₃ H ₂₅ N ₃ O ₂	255.3631											
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Halogen atoms	0.0000												
rotatable bonds	5.0000												
H-bond acceptors	4.0000												
H-bond donors	2.0000												
LogP	-1.0825												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-[3-(morpholin-4-yl)propyl]piperidine-4-carboxamide													

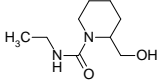
SS-3980	C ₁₂ H ₂₁ ClN ₂ O ₃	276.7658											
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Halogen atoms	1.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.5435												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-(chloroacetyl)-4-(tert-butoxycarbonyl)aminopiperidine													

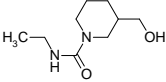
SS-3990	C ₁₂ H ₁₅ NO ₃	221.2583	
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		rotatable bonds	4.0000
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	1.4004
		LogS	TPSA
3-(3-(dimethylamino)-3-oxopropyl)benzoic acid			

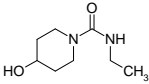
SS-3993	C ₆ H ₈ N ₂ O ₂ S	172.2069	
		Halogen atoms	0.0000
		rotatable bonds	3.0000
		H-bond acceptors	3.0000
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		LogP	1.0058
		LogS	TPSA
2-(1-methyl-1H-imidazol-2-ylthio)acetic acid			

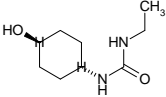
SS-3996	C ₅ H ₁₅ ClN ₂ O ₂ S	202.7045	
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		rotatable bonds	
		H-bond acceptors	3.0000
		H-bond donors	1.0000
		LogP	-1.0524
		LogS	TPSA
(N,N-dimethyl)-(3-aminopropyl)sulfonamide hydrochloride			

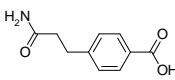
SS-3997	C ₉ H ₁₈ N ₂ O ₅	234.2542	
		Halogen atoms	0.0000
		rotatable bonds	5.0000
		H-bond acceptors	6.0000
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		LogP	-0.8545
		LogS	TPSA
5-amino-N,N-dimethylpentanamide oxalic acid salt			

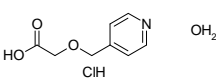
SS-3999	C ₉ H ₁₈ N ₂ O ₂	186.2560	
		Halogen atoms	0.0000
		rotatable bonds	2.0000
		H-bond acceptors	2.0000
		H-bond donors	2.0000
		LogP	0.1275
		LogS	TPSA
N-ethyl-2-(hydroxymethyl)piperidine-1-carboxamide			

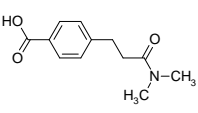
SS-4001	C ₉ H ₁₈ N ₂ O ₂	186.2560	
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		rotatable bonds	2.0000
		H-bond acceptors	2.0000
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		LogP	-0.1995
		LogS	TPSA
N-ethyl-3-(hydroxymethyl)piperidine-1-carboxamide			

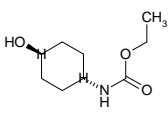
SS-4002	C ₈ H ₁₆ N ₂ O ₂	172.2289	
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		rotatable bonds	1.0000
		H-bond acceptors	2.0000
		H-bond donors	2.0000
		LogP	-0.6680
		LogS	TPSA
N-ethyl-4-hydroxypiperidine-1-carboxamide			

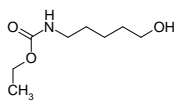
SS-4003	C ₉ H ₁₈ N ₂ O ₂	186.2560	
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		rotatable bonds	2.0000
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		H-bond donors	3.0000
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		LogS	TPSA
1-ethyl-3-((1r,4r)-4-hydroxycyclohexyl)urea			

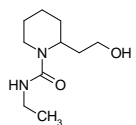
SS-4006	$C_{10}H_{11}NO_3$	193.2041											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	0.9074												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(2-carbamoyl)ethyl)benzoic acid													

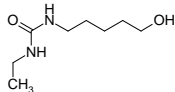
SS-4007	$C_8H_{12}ClNO_4$	221.6421											
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Halogen atoms	1.0000												
rotatable bonds													
H-bond acceptors	5.0000												
H-bond donors	2.0000												
LogP	0.4121												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(pyridin-4-ylmethoxy)acetic acid hydrochloride hydrate													

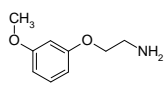
SS-4009	$C_{12}H_{15}NO_3$	221.2583											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	1.4004												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
4-(3-(dimethylamino)-3-oxopropyl)benzoic acid													

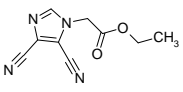
SS-4014	$C_9H_{17}NO_3$	187.2407											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>3.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.7087</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	0.7087	
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	0.7087												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl (1r,4r)-4-hydroxycyclohexylcarbamate													

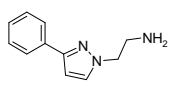
SS-4015	$C_8H_{17}NO_3$	175.2296											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>7.0000</td></tr> <tr><td>H-bond acceptors</td><td>3.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.6382</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	7.0000	H-bond acceptors	3.0000	H-bond donors	2.0000	LogP	0.6382	
Halogen atoms	0.0000												
rotatable bonds	7.0000												
H-bond acceptors	3.0000												
H-bond donors	2.0000												
LogP	0.6382												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
ethyl 5-hydroxypentylcarbamate													

SS-4016	$C_{10}H_{20}N_2O_2$	200.2831											
		<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>2.0000</td></tr> <tr><td>H-bond donors</td><td>2.0000</td></tr> <tr><td>LogP</td><td>0.1796</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	3.0000	H-bond acceptors	2.0000	H-bond donors	2.0000	LogP	0.1796	
Halogen atoms	0.0000												
rotatable bonds	3.0000												
H-bond acceptors	2.0000												
H-bond donors	2.0000												
LogP	0.1796												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
N-ethyl-2-(2-hydroxyethyl)piperidine-1-carboxamide													

SS-4017	$C_8H_{18}N_2O_2$	174.2449											
		<table border="1"> <tr><td>Halogen atoms</td><td>0.0000</td></tr> <tr><td>rotatable bonds</td><td>6.0000</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>-0.0118</td></tr> </table>	Halogen atoms	0.0000	rotatable bonds	6.0000	H-bond acceptors	2.0000	H-bond donors	3.0000	LogP	-0.0118	
Halogen atoms	0.0000												
rotatable bonds	6.0000												
H-bond acceptors	2.0000												
H-bond donors	3.0000												
LogP	-0.0118												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
1-ethyl-3-(5-hydroxypentyl)urea													

SS-4020	$C_9H_{13}NO_2$	167.2095											
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Halogen atoms	0.0000												
rotatable bonds	4.0000												
H-bond acceptors	3.0000												
H-bond donors	1.0000												
LogP	0.7506												
LogS	contact Key Organics for details	TPSA	contact Key Organics for details										
2-(3-methoxyphenoxy)ethanamine													

SS-4021	C ₉ H ₈ N ₄ O ₂	204.1897	
		Halogen atoms	
		0.0000	
		rotatable bonds	
		4.0000	
		H-bond acceptors	
5.0000			
H-bond donors	0.0000		
LogP	-0.1917		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
ethyl 2-(4,5-dicyano-1H-imidazol-1-yl)acetate			

SS-4022	C ₁₁ H ₁₃ N ₃	187.2464	
		Halogen atoms	
		0.0000	
		rotatable bonds	
		3.0000	
		H-bond acceptors	
2.0000			
H-bond donors	1.0000		
LogP	1.9134		
LogS	contact Key Organics for details	TPSA	contact Key Organics for details
1-aminoethyl-4-phenyl-pyrazole			