

# Azintamide

<b>Other names:</b>	2-(6-chloropyridazin-3-yl)sulfanyl-N,N-diethylacetamide
<b>Inchi:</b>	InChI=1S/C10H14ClN3OS/c1-3-14(4-2)10(15)7-16-9-6-5-8(11)12-13-9/h5-6H,3-4,7H2,1-
<b>InchiKey:</b>	SSLKKMZJCJBOML-UHFFFAOYSA-N
<b>Formula:</b>	C10H14ClN3OS
<b>SMILES:</b>	CCN(CC)C(=O)CSc1ccc(Cl)nn1
<b>Mol. weight [g/mol]:</b>	259.76

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Aqueous Solubility Prediction Method
log10ws	-1.72		Estimated Solubility Method
log10ws	-1.72		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.091		Crippen Method
mcvol	188.100	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>Aqueous and cosolvent solubility data for drug-like organic compounds:</b>	<a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/100-424-9/Azintamide.pdf>

Generated by Cheméo on 2024-05-17 21:13:25.874886107 +0000 UTC m=+18269654.795463419.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.