

# Thiazolo[5,4-d]pyrimidine, 5-amino-2-[(2-chloroethyl)thio]-7-(ethylamino)-

<b>Inchi:</b>	InChI=1S/C9H12ClN5S2/c1-2-12-6-5-7(15-8(11)14-6)17-9(13-5)16-4-3-10/h2-4H2,1H3,(
<b>InchiKey:</b>	BBJKZHFPFIPANV-UHFFFAOYSA-N
<b>Formula:</b>	C9H12ClN5S2
<b>SMILES:</b>	CCNc1nc(N)nc2sc(SCCCl)nc12
<b>Mol. weight [g/mol]:</b>	289.81
<b>CAS:</b>	93457-19-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	2.431		Crippen Method
mcvol	193.590	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C93457193&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93457193&amp;Units=SI</a>
<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>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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.chemeo.com/cid/54-070-4/Thiazolo-5-4-d-pyrimidine-5-amino-2-2-chloroethyl-thio-7-ethylamino.pdf>

Generated by Cheméo on 2024-04-27 21:08:25.363866545 +0000 UTC m=+16541354.284443861.

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