

4-Thiazolidinone, 3-amino-2-thioxo-

Other names:	N-Aminorhodanine 3-Aminorhodanine Rhodanine, 3-amino-
Inchi:	InChI=1S/C3H4N2OS2/c4-5-2(6)1-8-3(5)7/h1,4H2
InchiKey:	ZBUUHLDYMKTVLT-UHFFFAOYSA-N
Formula:	C3H4N2OS2
SMILES:	NN1C(=O)CSC1=S
Mol. weight [g/mol]:	148.21
CAS:	1438-16-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	-0.280		Crippen Method
mcvol	92.200	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1438160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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