

N-Methylrhodanine

Other names:	4-Thiazolidinone, 3-methyl-2-thioxo-Methylrhodanine Rhodanine, N-methyl-Rhodanine, 3-methyl- USAF T-2 3-Methylrhodanine NSC 14787 NSC 42903 NSC 65351 3-Methylrhodanide
Inchi:	InChI=1S/C4H5NOS2/c1-5-3(6)2-8-4(5)7/h2H2,1H3
InchiKey:	JKLZCQWVERBDEZ-UHFFFAOYSA-N
Formula:	C4H5NOS2
SMILES:	CN1C(=O)CSC1=S
Mol. weight [g/mol]:	147.22
CAS:	4807-55-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	0.476		Crippen Method
mvol	96.310	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C4807550&Units=SI

Legend

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

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