

Rhodanine, 5,5'-methylidynedi-

Inchi:	InChI=1S/C7H4N2O2S4/c10-4-2(14-6(12)8-4)1-3-5(11)9-7(13)15-3/h1,10H,(H,8,12)(H,9,
InchiKey:	AQWBSSESBGJSJPQ-IWQZZHSRSA-N
Formula:	C7H4N2O2S4
SMILES:	O=C1NC(=S)SC1=Cc1sc(=S)[nH]c1O
Mol. weight [g/mol]:	276.38
CAS:	28320-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	1.518		Crippen Method
mcvol	163.370	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=C28320436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/27-506-0/Rhodanine-5-5-methylidynedi.pdf>

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