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: AQWBSESBGJSJPQ-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