3H-1,2-Dithiol-3-one, 5-methyl-

Other names: 5-Methyl-3H-1,2-dithiol-3-one
Inchi: InChI=1S/C4H4OS2/c1-3-2-4(5)7-6-3/h2H,1H3
InchiKey: HKJJSYSMGYOWKY-UHFFFAOYSA-N
Formula: C4H4OS2
SMILES: Cc1cc(=O)ss1
Mol. weight [g/mol]: 132.20
CAS: 3620-08-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	1.478		Crippen Method
mcvol	86.330	ml/mol	McGowan Method
rinpol	1141.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3620084&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices