

Disulfide, bis(2-thenoyl)-

Inchi:	InChI=1S/C10H6O2S4/c11-9(7-3-1-5-13-7)15-16-10(12)8-4-2-6-14-8/h1-6H
InchiKey:	ZPWFFRLQFIXCDO-UHFFFAOYSA-N
Formula:	C10H6O2S4
SMILES:	O=C(SSC(=O)c1cccs1)c1cccs1
Mol. weight [g/mol]:	286.41
CAS:	116401-30-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	4.172		Crippen Method
mcvol	181.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/83-439-3/Disulfide-bis-2-thenoyl.pdf>

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