

Thiophene,3,3'-thiobis-

Other names:	Di-(3-thienyl)sulfide
Inchi:	InChI=1S/C8H6S3/c1-3-9-5-7(1)11-8-2-4-10-6-8/h1-6H
InchiKey:	NNPKTEYAZSRKAG-UHFFFAOYSA-N
Formula:	C8H6S3
SMILES:	c1cc(Sc2ccsc2)cs1
Mol. weight [g/mol]:	198.33
CAS:	3807-38-3

Physical Properties

Property code	Value	Unit	Source
ie	8.06	eV	NIST Webbook
log10ws	-3.40		Crippen Method
logp	3.961		Crippen Method
mcvol	133.710	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3807383&Units=SI
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

Legend

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

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