

Thiophene,2,2'-thiobis-

Other names: 2-(2-Thienylthio)thiophene
Inchi: InChI=1S/C8H6S3/c1-3-7(9-5-1)11-8-4-2-6-10-8/h1-6H
InchiKey: AKYIWBKPINOXJY-UHFFFAOYSA-N
Formula: C8H6S3
SMILES: c1csc(Sc2cccs2)c1
Mol. weight [g/mol]: 198.33
CAS: 3988-99-6

Physical Properties

Property code	Value	Unit	Source
ie	8.40	eV	NIST Webbook
log10ws	-3.40		Crippen Method
logp	3.961		Crippen Method
mcvol	133.710	ml/mol	McGowan Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3988996&Units=SI>

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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<https://www.chemeo.com/cid/54-174-9/Thiophene-2-2-thiobis.pdf>

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