

Thiophene, 2,2'-dithiobis-

Other names:	Disulfide, 2-thienyl 2-Thienyl disulfide bis(2-Thienyl)disulfide 2-(2-Thienyldisulfanyl)thiophene bis(2-Thienyl) disulphide 2-thiophen-2-ylsulfanylthiophene
Inchi:	InChI=1S/C8H6S4/c1-3-7(9-5-1)11-12-8-4-2-6-10-8/h1-6H
InchiKey:	YOLFWWMPGNMXFI-UHFFFAOYSA-N
Formula:	C8H6S4
SMILES:	<chem>c1csc(SSc2cccs2)c1</chem>
Mol. weight [g/mol]:	230.39
CAS:	6911-51-9

Physical Properties

Property code	Value	Unit	Source
ie	7.50	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-4.28		Crippen Method
logp	4.609		Crippen Method
mcvol	150.060	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6911519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

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/56-510-3/Thiophene-2-2-dithiobis.pdf>

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