Thiophene, 2-methyl-3-(methylthio)

Other names:	2-methyl-3-(methylthio)thiophene
Inchi:	InChI=1S/C6H8S2/c1-5-6(7-2)3-4-8-5/h3-4H,1-2H3
InchiKey:	MRVFTOBCUYZFSE-UHFFFAOYSA-N
Formula:	C6H8S2
SMILES:	CSc1ccsc1C
Mol. weight [g/mol]:	144.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Crippen Method
logp	2.778		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
rinpol	1141.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1144.00		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=R90797&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

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