

Thiophene, 3-(methylthio)-

Other names:	3-(Methylthio)thiophene 3-(Methylsulfanyl)thiophene 3-Thienylmethylsulfide Methyl 3-thienyl sulfide 3-(methylthio)-3-thiophene
Inchi:	InChI=1S/C5H6S2/c1-6-5-2-3-7-4-5/h2-4H,1H3
InchiKey:	OTYBVBDWIKXFDO-UHFFFAOYSA-N
Formula:	C5H6S2
SMILES:	CS _c 1ccsc1
Mol. weight [g/mol]:	130.23
CAS:	20731-74-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	2.470		Crippen Method
mcvol	94.550	ml/mol	McGowan Method
rinpol	1070.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1635.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20731742&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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