

Thiophene, 2-(methylthio)-

Other names:	2-(Methylthio)thiophene 2-(Methylsulfanyl)thiophene
Inchi:	InChI=1S/C5H6S2/c1-6-5-3-2-4-7-5/h2-4H,1H3
InchiKey:	ZLSMPEVZXWDWEK-UHFFFAOYSA-N
Formula:	C5H6S2
SMILES:	CSc1cccs1
Mol. weight [g/mol]:	130.23
CAS:	5780-36-9

Physical Properties

Property code	Value	Unit	Source
ie	8.63 ± 0.05	eV	NIST Webbook
ie	8.10 ± 0.05	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	2.470		Crippen Method
mcvol	94.550	ml/mol	McGowan Method
rinpol	1020.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1036.00		NIST Webbook

Sources

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=C5780369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
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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