

Thiophene,2-methyl-5-(methylthio)-

Other names:	Thiophene,2-methyl-5-(methylthiol)-
Inchi:	InChI=1S/C6H8S2/c1-5-3-4-6(7-2)8-5/h3-4H,1-2H3
InchiKey:	VSUGUKXAAPOFPQ-UHFFFAOYSA-N
Formula:	C6H8S2
SMILES:	CSc1ccc(C)s1
Mol. weight [g/mol]:	144.26
CAS:	40990-29-2

Physical Properties

Property code	Value	Unit	Source
ie	8.13 ± 0.05	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.778		Crippen Method
mcvol	108.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40990292&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

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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