

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

Other names:	Methyl 5-methylfuryl sulfide 2-Methyl-5-(methylthio)furan 5-Methyl-2-(methylthio)furan
Inchi:	InChI=1S/C6H8OS/c1-5-3-4-6(7-5)8-2/h3-4H,1-2H3
InchiKey:	RESBOJMQOGJOMW-UHFFFAOYSA-N
Formula:	C6H8OS
SMILES:	CSc1ccc(C)o1
Mol. weight [g/mol]:	128.19
CAS:	13678-59-6

Physical Properties

Property code	Value	Unit	Source
ie	8.15 ± 0.05	eV	NIST Webbook
log10ws	-6.42		Crippen Method
logp	2.310		Crippen Method
mcvol	98.160	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13678596&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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<https://www.chemeo.com/cid/50-297-7/Furan-2-methyl-5-methylthio.pdf>

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