

Furan, 2-[(methylthio)methyl]-

Other names:	Furfuryl methyl sulfide 2-Furfuryl methyl sulfide 2-Furfuryl methyl sulphide 2-(Methylthio)methylfuran Methyl 2-furfuryl sulfide 2-[(Methylsulfanyl)methyl]furan
Inchi:	InChI=1S/C6H8OS/c1-8-5-6-3-2-4-7-6/h2-4H,5H2,1H3
InchiKey:	SKSFHXVDHVKIBN-UHFFFAOYSA-N
Formula:	C6H8OS
SMILES:	CSCc1ccco1
Mol. weight [g/mol]:	128.19
CAS:	1438-91-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	2.143		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinpol	988.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	998.00		NIST Webbook

rinpol	980.00	NIST Webbook
rinpol	972.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	990.00	NIST Webbook
rinpol	984.00	NIST Webbook
ripol	1492.00	NIST Webbook
ripol	1493.00	NIST Webbook
ripol	1493.00	NIST Webbook
ripol	1485.00	NIST Webbook
ripol	1476.00	NIST Webbook
ripol	1480.00	NIST Webbook
ripol	1503.00	NIST Webbook
ripol	1485.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1506.00	NIST Webbook
ripol	1502.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1450.00	NIST Webbook
ripol	1465.00	NIST Webbook
ripol	1481.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1481.00	NIST Webbook
ripol	1492.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1438911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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