

Furan, 2-[[1-methylethyl)thio]methyl]-

Other names:	Furan, 2-[(isopropylthio)methyl]- Isopropyl furfuryl sulfide 2-[[1-Methylethyl)thio]methyl]furan Furfuryl isopropyl sulfide 2-(propan-2-ylsulfanylmethyl)furan
Inchi:	InChI=1S/C8H12OS/c1-7(2)10-6-8-4-3-5-9-8/h3-5,7H,6H2,1-2H3
InchiKey:	WCHRNAKORAINOJ-UHFFFAOYSA-N
Formula:	C8H12OS
SMILES:	CC(C)SCc1ccco1
Mol. weight [g/mol]:	156.25
CAS:	1883-78-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	2.921		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
rinpol	1116.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1113.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1883789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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