

2-methyl-3-(methylthio)furan

Other names:	Furan, 2-methyl-3-(methylthio)
Inchi:	InChI=1S/C6H8OS/c1-5-6(8-2)3-4-7-5/h3-4H,1-2H3
InchiKey:	OQVAOEIMSKZGAL-UHFFFAOYSA-N
Formula:	C6H8OS
SMILES:	CSc1ccoc1C
Mol. weight [g/mol]:	128.19
CAS:	63012-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	2.310		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
ripol	944.00		NIST Webbook
ripol	963.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	910.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	925.00		NIST Webbook
ripol	933.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	947.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1356.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C63012975&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

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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