

2-Methyl-3-(methyldithio)furan

Other names:	2-methyl-3-methyldithio-furane Methyl 2-methyl-3-furyl disulfide Furan, 2-methyl-3-(methyldithio) (2-Methylfuryl-3)methyl disulfide
Inchi:	InChI=1S/C6H8OS2/c1-5-6(9-8-2)3-4-7-5/h3-4H,1-2H3
InchiKey:	SRUTWBWLFKSTIS-UHFFFAOYSA-N
Formula:	C6H8OS2
SMILES:	CSSc1ccoc1C
Mol. weight [g/mol]:	160.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.958		Crippen Method
mcvol	114.510	ml/mol	McGowan Method
rinpol	1153.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1178.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1651.00		NIST Webbook

ripol	1667.00	NIST Webbook
ripol	1668.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1670.00	NIST Webbook
ripol	1655.00	NIST Webbook
ripol	1667.00	NIST Webbook
ripol	1663.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1667.00	NIST Webbook
ripol	1669.00	NIST Webbook
ripol	1654.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1615.00	NIST Webbook
ripol	1668.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65505171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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