Furan, 2-[(methyldithio)methyl]-

Other names:	Furfuryl methyl disulfide
	2-Furfuryl methyl disulfide
	2-Furfuryl methyl disulphide
	2-[(Methyldithio)methyl]furan
	Furfuryl methyl disulphide
Inchi:	InChI=1S/C6H8OS2/c1-8-9-5-6-3-2-4-7-6/h2-4H,5H2,1H3
InchiKey:	CLSLQQCDHOZMDT-UHFFFAOYSA-N
Formula:	C6H8OS2
SMILES:	CSSCc1ccco1
Mol. weight [g/mol]:	160.26
CAS:	57500-00-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.26		Crippen Method
logp	2.791		Crippen Method
mcvol	114.510	ml/mol	McGowan Method
rinpol	1188.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1199.00		NIST Webbook
ripol	1804.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1804.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57500002&Units=SI

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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