

furfuryl 2-methyl-3-furyl disulfide

Other names:	Furan, 3-[(2-furanylmethyl)dithio]-2-methyl-2-furfuryl 2-methyl-3-furyl disulfide
Inchi:	InChI=1S/C10H10O2S2/c1-8-10(4-6-11-8)14-13-7-9-3-2-5-12-9/h2-6H,7H2,1H3
InchiKey:	FVCZDGBJCOHRKY-UHFFFAOYSA-N
Formula:	C10H10O2S2
SMILES:	Cc1occc1SSCc1ccco1
Mol. weight [g/mol]:	226.31
CAS:	109537-55-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.14		Crippen Method
logp	4.122		Crippen Method
mccvol	157.280	ml/mol	McGowan Method
rinpol	1620.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2347.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109537555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ripol:	Polar retention indices

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