

Furfuryl sulfide

Other names:	Difurfuryl sulfide Furan, 2,2'-[thiobis(methylene)]bis- 2-((2-Furylmethyl)sulfanyl)methyl)furan 2-Difurfuryl sulfide bis(2-Furylmethyl) sulfide bis-Furfuryl sulfide di-2-Furfuryl sulfide 2,2'-[thiobis(methylene)]bisfuran
Inchi:	InChI=1S/C10H10O2S/c1-3-9(11-5-1)7-13-8-10-4-2-6-12-10/h1-6H,7-8H2
InchiKey:	UYLKDZXJEKFFHJ-UHFFFAOYSA-N
Formula:	C10H10O2S
SMILES:	<chem>c1coc(CSCc2ccco2)c1</chem>
Mol. weight [g/mol]:	194.25
CAS:	13678-67-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.23		Crippen Method
logp	3.306		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
rinpol	1416.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1463.00		NIST Webbook
ripol	2223.00		NIST Webbook
ripol	2178.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13678676&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
ripol:	Polar retention indices

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