

2-furfuryl 2-oxo-3-butyl disulfide

Other names:	3-[(2-Furylmethyl)dithio]-2-butanone
Inchi:	InChI=1S/C9H12O2S2/c1-7(10)8(2)13-12-6-9-4-3-5-11-9/h3-5,8H,6H2,1-2H3
InchiKey:	LOGIPTDAOGQBBJ-UHFFFAOYSA-N
Formula:	C9H12O2S2
SMILES:	CC(=O)C(C)SSCc1ccc1
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.91		Crippen Method
logp	3.138		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
rinpol	1589.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1589.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2352.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365960&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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