2-furfuryl 2-oxo-propyl disulfide

Inchi:	InChI=1S/C8H10O2S2/c1-7(9)5-11-12-6-8-3-2-4-10-8/h2-4H,5-6H2,1H3
InchiKey:	IRWUGOPPCRXHIM-UHFFFAOYSA-N
Formula:	C8H10O2S2
SMILES:	CC(=O)CSSCc1ccco1
Mol. weight [g/mol]:	202.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.38		Crippen Method
logp	2.750		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
rinpol	1540.00		NIST Webbook
ripol	2400.00		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=R224069&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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