

2-furfuryl hydrodisulfide

Inchi: InChI=1S/C5H6OS2/c7-8-4-5-2-1-3-6-5/h1-3,7H,4H2
InchiKey: RKOZKDPRABIQQY-UHFFFAOYSA-N
Formula: C5H6OS2
SMILES: SSCc1cccc1
Mol. weight [g/mol]: 146.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	2.358		Crippen Method
mcvol	100.420	ml/mol	McGowan Method
rinpol	1121.00		NIST Webbook
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Sources

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=R219928&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/66-148-5/2-furfuryl-hydrodisulfide.pdf>

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