

methylfurfuryl disulfide

Inchi: InChI=1S/C5H6OS2/c1-7-8-5-3-2-4-6-5/h2-4H,1H3
InchiKey: VWBDHVFAXXPCEX-UHFFFAOYSA-N
Formula: C5H6OS2
SMILES: CSSc1cccc1
Mol. weight [g/mol]: 146.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.650		Crippen Method
mcvol	100.420	ml/mol	McGowan Method
rinsol	1199.00		NIST Webbook
rinsol	1182.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R245873&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/96-753-0/methylfurfuryl-disulfide.pdf>

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