

5-methylfurfuryl methyl disulfide

Inchi: InChI=1S/C7H10OS2/c1-6-3-4-7(8-6)5-10-9-2/h3-4H,5H2,1-2H3
InchiKey: NVRIWCPYIZINPN-UHFFFAOYSA-N
Formula: C7H10OS2
SMILES: CSSCc1ccc(C)o1
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.74		Crippen Method
logp	3.099		Crippen Method
mcvol	128.600	ml/mol	McGowan Method

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=R489791&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/98-648-5/5-methylfurfuryl-methyl-disulfide.pdf>

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