

3-(Methylthio)methylfuran

Inchi: InChI=1S/C6H8OS/c1-8-5-6-2-3-7-4-6/h2-4H,5H2,1H3
InchiKey: QMDWXIARGAQRDV-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CSCc1ccoc1
Mol. weight [g/mol]: 128.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	2.143		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
ripol	1463.00		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=R319741&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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<https://www.chemeo.com/cid/81-042-5/3-Methylthio-methylfuran.pdf>

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