

2-Methylfuran-3-thiol

Inchi: InChI=1S/C5H6OS/c1-4-2-3-6-5(4)7/h2-3,7H,1H3
InchiKey: TYOASUAPMVRQOA-UHFFFAOYSA-N
Formula: C5H6OS
SMILES: Cc1ccoc1S
Mol. weight [g/mol]: 114.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	1.877		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R613662&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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<https://www.chemeo.com/cid/88-082-4/2-Methylfuran-3-thiol.pdf>

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