

3-Furanthiol

Inchi: InChI=1S/C4H4OS/c6-4-1-2-5-3-4/h1-3,6H
InchiKey: MWFFRFMPYAKXEY-UHFFFAOYSA-N
Formula: C4H4OS
SMILES: Sc1ccoc1
Mol. weight [g/mol]: 100.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	1.568		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
rinpol	746.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	746.00		NIST Webbook

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=R69699&Units=SI>

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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