

Thiophene-2-ol

Inchi: InChI=1S/C4H4OS/c5-4-2-1-3-6-4/h1-3,5H
InchiKey: WZMPOCLULGAHJR-UHFFFAOYSA-N
Formula: C4H4OS
SMILES: Oc1cccs1
Mol. weight [g/mol]: 100.14
CAS: 17236-58-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.78		Crippen Method
logp	1.454		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
rinpol	956.00		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=C17236587&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/87-967-3/Thiophene-2-ol.pdf>

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