

3,4-Dimethylthiophene-2-thiol

Inchi: InChI=1S/C6H8S2/c1-4-3-8-6(7)5(4)2/h3,7H,1-2H3
InchiKey: QHTDBIYIHXBQY-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: Cc1csc(S)c1C
Mol. weight [g/mol]: 144.26
CAS: 153001-04-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.654		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
rinpola	1193.50		NIST Webbook
rinpola	1193.50		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C153001048&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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