

3-methyl-2-thiophenemethanethiol

Inchi: InChI=1S/C6H8S2/c1-5-2-3-8-6(5)4-7/h2-3,7H,4H2,1H3
InchiKey: SOQJSJRXHJTTOH-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: Cc1ccsc1CS
Mol. weight [g/mol]: 144.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.486		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R336419&Units=SI>

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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