2-(1-mercaptoethyl)thiophene

Inchi: InChI=1S/C6H8S2/c1-5(7)6-3-2-4-8-6/h2-5,7H,1H3
InchiKey: NCCCTQRHFVSOMP-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: CC(S)c1cccs1
Mol. weight [g/mol]: 144.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	2.739		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
rinpol	1136.00		NIST Webbook
rinpol	1136.00		NIST Webbook
ripol	1655.00		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=R225582&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
ripol: Polar retention indices

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