2-Thienylmethanethiol, 5-methyl

Inchi: InChI=1S/C6H8S2/c1-5-2-3-6(4-7)8-5/h2-3,7H,4H2,1H3
InchiKey: VAZXIFBACHWZIJ-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: Cc1ccc(CS)s1
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
rinpol	1179.00		NIST Webbook
rinpol	1183.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R89388&Units=SI
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

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.