2-thienylethylthiomethane

Inchi: InChI=1S/C7H10S2/c1-2-8-6-7-4-3-5-9-7/h3-5H,2,6H2,1H3
InchiKey: AFCJCLDOMXGCMV-UHFFFAOYSA-N
Formula: C7H10S2
SMILES: CCSCc1cccs1
Mol. weight [g/mol]: 158.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	3.001		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinpol	1251.00		NIST Webbook
rinpol	1251.00		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=R156397&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

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