2-(propylsulfanyl)thiophene

Inchi: InChI=1S/C8H12S2/c1-2-5-9-7-8-4-3-6-10-8/h3-4,6H,2,5,7H2,1H3
InchiKey: ZNIHSLHDQPGMPH-UHFFFAOYSA-N
Formula: C8H12S2
SMILES: CCCSCc1cccs1
Mol. weight [g/mol]: 172.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	3.391		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R259357&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.