2-(1-PROPENYLTHIO)THIOPHENE

Inchi: InChI=1S/C7H8S2/c1-2-5-8-7-4-3-6-9-7/h2-6H,1H3/b5-2-
InchiKey: KHVVAPOSLPACCP-GORDUTHDSA-N
Formula: C7H8S2
SMILES: C/C=C/Sc1cccs1
Mol. weight [g/mol]: 156.28

Physical Properties

Property code	Value	Unit	Source
ie	7.89	eV	Cheméo Relay (1.0)
logp	3.374		Crippen Method
mcvol	118.430	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C199480756&Units=SI

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume