Thiophene, 3-(1-methylethyl)thio

Inchi: InChI=1S/C7H10S2/c1-6(2)9-7-3-4-8-5-7/h3-6H,1-2H3
InchiKey: IUWNGVPRUJILJM-UHFFFAOYSA-N
Formula: C7H10S2
SMILES: CC(C)Sc1ccsc1
Mol. weight [g/mol]: 158.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	3.249		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinpol	1168.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1161.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R57765&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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