Thiophene, 2-(1-methylpropyl)thio

Inchi: InChI=1S/C8H12S2/c1-3-7(2)10-8-5-4-6-9-8/h4-7H,3H2,1-2H3
InchiKey: MGLRFPVDQZHEOJ-UHFFFAOYSA-N
Formula: C8H12S2
SMILES: CCC(C)Sc1cccs1
Mol. weight [g/mol]: 172.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	3.639		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
rinpol	1250.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1246.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R57729&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

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