

Thiophene, 4-methyl-2-propyl

Other names: 2-Propyl-4-methylthiophene
Inchi: InChI=1S/C8H12S/c1-3-4-8-5-7(2)6-9-8/h5-6H,3-4H2,1-2H3
InchiKey: MJEUTQPVYUFHCU-UHFFFAOYSA-N
Formula: C8H12S
SMILES: CCCc1cc(C)cs1
Mol. weight [g/mol]: 140.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	3.009		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook

Sources

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=R41883&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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