

Thiophene, 2-ethyl-3,5-dimethyl

Other names: 2-Ethyl-3,5-dimethylthiophene
Inchi: InChI=1S/C8H12S/c1-4-8-6(2)5-7(3)9-8/h5H,4H2,1-3H3
InchiKey: XXLBZDCPBSGOJR-UHFFFAOYSA-N
Formula: C8H12S
SMILES: CCc1sc(C)cc1C
Mol. weight [g/mol]: 140.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.927		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1044.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1045.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41801&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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