

Thiophene, 2-butyl-3,5-dimethyl

Other names: 2-Butyl-3,5-dimethylthiophene
Inchi: InChI=1S/C10H16S/c1-4-5-6-10-8(2)7-9(3)11-10/h7H,4-6H2,1-3H3
InchiKey: MRLGYUYIBGNGBZ-UHFFFAOYSA-N
Formula: C10H16S
SMILES: CCCCC1sc(C)cc1C
Mol. weight [g/mol]: 168.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	3.708		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R41744&Units=SI>

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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