Thiophene, 5-butyl-2,3-dimethyl

Other names: 5-Butyl-2,3-dimethylthiophene
Inchi: InChI=1S/C10H16S/c1-4-5-6-10-7-8(2)9(3)11-10/h7H,4-6H2,1-3H3
InchiKey: FBJKLGICJXNWFB-UHFFFAOYSA-N
Formula: C10H16S
SMILES: CCCCc1cc(C)c(C)s1
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	1245.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1245.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41605&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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