

4-Methyl-2-nonylbenzo[b]thiophene

Other names: Benzo[b]thiophene, 4-methyl-2-nonyl
Inchi: InChI=1S/C18H26S/c1-3-4-5-6-7-8-9-12-16-14-17-15(2)11-10-13-18(17)19-16/h10-11,13
InchiKey: ZBIKGTUDZAGMFZ-UHFFFAOYSA-N
Formula: C18H26S
SMILES: CCCCCCCCCc1cc2c(C)cccc2s1
Mol. weight [g/mol]: 274.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	6.503		Crippen Method
mcvol	241.910	ml/mol	McGowan Method
rinpol	2207.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2217.20		NIST Webbook
rinpol	2207.00		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=R41637&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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