

Anthro[2,1-b]thiophene, 1-methyl

Inchi: InChI=1S/C17H12S/c1-11-10-18-16-7-6-14-8-12-4-2-3-5-13(12)9-15(14)17(11)16/h2-10H
InchiKey: ATNNEKZLGVHIPV-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1csc2ccc3cc4ccccc4cc3c12
Mol. weight [g/mol]: 248.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinpol	416.04		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R642452&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

Latest version available from:

<https://www.chemeo.com/cid/74-476-2/Anthro-2-1-b-thiophene-1-methyl.pdf>

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