

Anthro[2,1-b]thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-12-10-15-13(9-11(12)3-1)5-6-16-14(15)7-8-17-16/h1-10H
InchiKey: PAYSBLPSJQBEJR-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2cc3c(ccc4sccc43)cc2c1
Mol. weight [g/mol]: 234.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	5.208		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
rinpol	399.27		NIST Webbook
rinpol	399.27		NIST Webbook

Sources

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=R642447&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/73-984-9/Anthro-2-1-b-thiophene.pdf>

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