

Anthra(2,3-b)thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-12-8-15-10-16-13(5-6-17-16)9-14(15)7-11(12)3-1/h1-10H
InchiKey: QOOSFVFWJXNCTP-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2cc3cc4sccc4cc3cc2c1
Mol. weight [g/mol]: 234.32
CAS: 22108-55-0

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	407.57		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C22108550&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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<https://www.chemeo.com/cid/78-375-0/Anthra-2-3-b-thiophene.pdf>

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