

Phenanthro[2,3-b]thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-14-11(3-1)5-6-12-10-16-13(7-8-17-16)9-15(12)14/h1-10H
InchiKey: PUDWJHJHVOOWEE-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2c(c1)ccc1cc3sccc3cc12
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	400.80		NIST Webbook
rinpol	400.80		NIST Webbook
rinpol	402.13		NIST Webbook
rinpol	402.19		NIST Webbook
rinpol	400.80		NIST Webbook
rinpol	399.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R21706&Units=SI>
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>

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/73-982-1/Phenanthro-2-3-b-thiophene.pdf>

Generated by Cheméo on 2024-04-26 08:59:51.203888602 +0000 UTC m=+16411240.124465918.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.