

Phenanthro[4,3-b]thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-14-11(3-1)5-6-12-7-8-13-9-10-17-16(13)15(12)14/h1-10H
InchiKey: HVDXWEZIEYUOMI-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2c(c1)ccc1ccc3ccsc3c12
Mol. weight [g/mol]: 234.32
CAS: 195-68-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	5.208		Crippen Method
mccvol	174.810	ml/mol	McGowan Method
rinpol	395.34		NIST Webbook
rinpol	394.64		NIST Webbook
rinpol	395.16		NIST Webbook
rinpol	395.03		NIST Webbook
rinpol	395.10		NIST Webbook
rinpol	394.30		NIST Webbook
rinpol	395.10		NIST Webbook
rinpol	395.20		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=C195686&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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