

Phenanthro[9,10-b]thiophene

Inchi: InChI=1S/C16H10S/c1-2-7-13-11(5-1)12-6-3-4-8-14(12)16-15(13)9-10-17-16/h1-10H
InchiKey: OGOOBRWCZLKZSV-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2c(c1)c1ccccc1c1sccc21
Mol. weight [g/mol]: 234.32

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	394.64		NIST Webbook
rinpol	394.90		NIST Webbook
rinpol	394.00		NIST Webbook
rinpol	394.80		NIST Webbook
rinpol	394.64		NIST Webbook
rinpol	394.64		NIST Webbook
rinpol	394.96		NIST Webbook
rinpol	394.80		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R111507&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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