

Phenanthro(3,2-b)thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-14-11(3-1)5-6-12-9-13-7-8-17-16(13)10-15(12)14/h1-10H
InchiKey: BKDNKFGDTSYPHA-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2c(c1)ccc1cc3ccsc3cc12
Mol. weight [g/mol]: 234.32
CAS: 224-10-2

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	401.78		NIST Webbook
rinpol	401.52		NIST Webbook
rinpol	401.89		NIST Webbook
rinpol	401.60		NIST Webbook
rinpol	401.60		NIST Webbook
rinpol	401.49		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C224102&Units=SI>

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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