Phenanthro(3,4-b)thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-13-11(3-1)5-6-12-7-8-15-14(16(12)13)9-10-17-15/h1-10H
InchiKey: XRJUVKFVUBGLMG-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2c(c1)ccc1ccc3sccc3c12
Mol. weight [g/mol]: 234.32
CAS: 195-52-8

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	396.46		NIST Webbook
rinpol	396.43		NIST Webbook
rinpol	396.70		NIST Webbook
rinpol	396.70		NIST Webbook
rinpol	396.88		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C195528&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices