Phenanthro(2,1-b)thiophene

Inchi: InChI=1S/C16H10S/c1-2-4-12-11(3-1)5-6-14-13(12)7-8-16-15(14)9-10-17-16/h1-10H
InchiKey: WYAKNOROQVZSDA-UHFFFAOYSA-N
Formula: C16H10S
SMILES: c1ccc2c(c1)ccc1c3ccsc3ccc21
Mol. weight [g/mol]: 234.32
CAS: 219-25-0

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	400.75		NIST Webbook
rinpol	399.58		NIST Webbook
rinpol	400.59		NIST Webbook
rinpol	400.75		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C219250&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