

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:	XRJUVKFKVUBGLMG-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

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