3-Methylphenanthro[9,10-b]thiophene

Other names: Phenanthro[9,10-b]thiophene, 3-methyl
Inchi: InChI=1S/C17H12S/c1-11-10-18-17-15-9-5-3-7-13(15)12-6-2-4-8-14(12)16(11)17/h2-10H
InchiKey: AKGGNOYSWJSWNW-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1csc2c3ccccc3c3ccccc3c12
Mol. weight [g/mol]: 248.34
CAS: 82420-70-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinpol	415.83		NIST Webbook
rinpol	417.70		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C82420700&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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