

10-Methylphenanthro[2,1-b]thiophene

Other names:	Phenanthro[2,1-b]thiophene, 10-methyl
Inchi:	InChI=1S/C17H12S/c1-11-10-16-14(8-9-18-16)15-7-6-12-4-2-3-5-13(12)17(11)15/h2-10H
InchiKey:	ZJUVQEAZKUGHFR-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	<chem>Cc1cc2sccc2c2ccc3ccccc3c12</chem>
Mol. weight [g/mol]:	248.34
CAS:	79966-04-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinsol	422.14		NIST Webbook
rinsol	422.14		NIST Webbook

Sources

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=C79966044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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