11-Methylbenzo[b]naphtho[2,3-d]thiophene

Other names: Benzo[b]naphtho[2,3-d]thiophene, 11-methyl
Benzo[b]naphtho[2,3]thiophene, 11-methyl
Inchi: InChI=1S/C17H12S/c1-11-13-7-3-2-6-12(13)10-16-17(11)14-8-4-5-9-15(14)18-16/h2-10H
InchiKey: BXBYDPRWMFDDSH-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1c2ccccc2cc2sc3ccccc3c12
Mol. weight [g/mol]: 248.34
CAS: 79966-33-9

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	422.85		NIST Webbook
rinpol	421.93		NIST Webbook
rinpol	421.93		NIST Webbook
rinpol	420.71		NIST Webbook
rinpol	420.71		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79966339&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices