10-Methylbenzo[b]naphtho[2,1-d]thiophene

Other names: Benzo[b]naphtho[2,1-d]thiophene, 10-methyl
Benzo[b]naphtho[2,1]thiophene, 10-methyl
Inchi: InChI=1S/C17H12S/c1-11-5-4-8-14-15-10-9-12-6-2-3-7-13(12)17(15)18-16(11)14/h2-10H
InchiKey: ALSLOOZOIWFNDC-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1cccc2c1sc1c3ccccc3ccc21
Mol. weight [g/mol]: 248.34
CAS: 83821-58-3

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	403.21		NIST Webbook
rinpol	404.28		NIST Webbook
rinpol	403.12		NIST Webbook
rinpol	403.21		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=C83821583&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices