Benzo[b]naphtho[1,2-d]thiophene, 10-methyl

Other names: Benzo[b]naphtho[1,2]thiophene, 10-methyl
Inchi: InChI=1S/C17H12S/c1-11-6-8-15-14(10-11)17-13-5-3-2-4-12(13)7-9-16(17)18-15/h2-10H
InchiKey: HRWDTHDOUKGIJR-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1ccc2sc3ccc4ccccc4c3c2c1
Mol. weight [g/mol]: 248.34

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	409.04		NIST Webbook
rinpol	407.23		NIST Webbook
rinpol	407.23		NIST Webbook
rinpol	409.04		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R21176&Units=SI

Legend

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