Benzo[b]naphtho[2,1-d]thiophene, 7-methyl

Other names: Benzo[b]naphtho[2,1]thiophene, 7-methyl
Inchi: InChI=1S/C17H12S/c1-11-5-4-8-15-16(11)14-10-9-12-6-2-3-7-13(12)17(14)18-15/h2-10H
InchiKey: QUYZXKBGOBBUCR-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1cccc2sc3c4ccccc4ccc3c12
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	411.03		NIST Webbook
rinpol	412.08		NIST Webbook
rinpol	412.08		NIST Webbook
rinpol	411.03		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=R21251&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