Benzo[b]naphtho[2,3]thiophene, 4-methyl

Other names: Benzo[b]naphtho[2,3-d]thiophene, 4-methyl
Inchi: InChI=1S/C17H12S/c1-11-5-4-8-14-15-9-12-6-2-3-7-13(12)10-16(15)18-17(11)14/h2-10H
InchiKey: YTNVYFJVEVMZDG-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1cccc2c1sc1cc3ccccc3cc12
Mol. weight [g/mol]: 248.34
CAS: 36821-08-6

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	411.60		NIST Webbook
rinpol	410.66		NIST Webbook
rinpol	411.60		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36821086&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