

Benzo[b]naphtho[2,3]thiophene, 1-methyl

Inchi: InChI=1S/C17H12S/c1-11-5-4-8-15-17(11)14-9-12-6-2-3-7-13(12)10-16(14)18-15/h2-10H
InchiKey: OFIFZSIDYJOJDZ-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1cccc2sc3cc4ccccc4cc3c12
Mol. weight [g/mol]: 248.34
CAS: 83656-85-3

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	415.54		NIST Webbook
rinpol	415.54		NIST Webbook
rinpol	414.47		NIST Webbook
rinpol	414.47		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C83656853&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

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