

Benzo[b]naphtho[2,1]thiophene, 6-methyl

Other names: Benzo[b]naphtho[2,1-d]thiophene, 6-methyl
Inchi: InChI=1S/C17H12S/c1-11-10-12-6-2-3-7-13(12)17-16(11)14-8-4-5-9-15(14)18-17/h2-10H
InchiKey: DAPKAZOYQHFTNG-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1cc2ccccc2c2sc3ccccc3c12
Mol. weight [g/mol]: 248.34
CAS: 84258-70-8

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	410.31		NIST Webbook
rinpol	411.71		NIST Webbook
rinpol	410.58		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C84258708&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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