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

Other names: Benzo[b]naphtho[2,1]thiophene, 1-methyl
Inchi: InChI=1S/C17H12S/c1-11-5-4-6-12-9-10-14-13-7-2-3-8-15(13)18-17(14)16(11)12/h2-10H
InchiKey: WRJGYDAQUXWJRB-UHFFFAOYSA-N
Formula: C17H12S
SMILES: Cc1cccc2ccc3c4ccccc4sc3c12
Mol. weight [g/mol]: 248.34
CAS: 4567-41-3

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	414.62		NIST Webbook
rinpol	413.97		NIST Webbook
rinpol	413.97		NIST Webbook
rinpol	412.97		NIST Webbook
rinpol	412.97		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4567413&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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