1,7-Dimethyldibenzothiophene

Other names: Dibenzothiophene, 1,7-dimethyl
Inchi: InChI=1S/C14H12S/c1-9-6-7-11-13(8-9)15-12-5-3-4-10(2)14(11)12/h3-8H,1-2H3
InchiKey: VFQYQNKOTDCRKH-UHFFFAOYSA-N
Formula: C14H12S
SMILES: Cc1ccc2c(c1)sc1cccc(C)c12
Mol. weight [g/mol]: 212.31
CAS: 89816-53-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.79		Crippen Method
logp	4.671		Crippen Method
mcvol	166.090	ml/mol	McGowan Method
rinpol	337.21		NIST Webbook
rinpol	338.93		NIST Webbook
rinpol	339.36		NIST Webbook
rinpol	335.55		NIST Webbook
rinpol	339.40		NIST Webbook
rinpol	337.21		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89816535&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