

1,9-dimethyl-dibenzothiophene

Other names:	Dibenzothiophene, 1,9-dimethyl
Inchi:	InChI=1S/C14H12S/c1-9-5-3-7-11-13(9)14-10(2)6-4-8-12(14)15-11/h3-8H,1-2H3
InchiKey:	DGUACJDPTAAFMP-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	<chem>Cc1cccc2sc3cccc(C)c3c12</chem>
Mol. weight [g/mol]:	212.31

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	339.49		NIST Webbook
rinpol	339.49		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R67300&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

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