

2,4,8-trimethyl-dibenzothiophene

Other names:	Dibenzothiophene, 2,4,8-trimethyl
Inchi:	InChI=1S/C15H14S/c1-9-4-5-14-12(7-9)13-8-10(2)6-11(3)15(13)16-14/h4-8H,1-3H3
InchiKey:	FEQHEOIAYXXUHR-UHFFFAOYSA-N
Formula:	C15H14S
SMILES:	<chem>Cc1ccc2sc3c(C)cc(C)cc3c2c1</chem>
Mol. weight [g/mol]:	226.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	4.980		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	347.99		NIST Webbook
rinpol	345.76		NIST Webbook

Sources

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=R193009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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