

4-ethyl,6-methyl-dibenzothiophene

Other names:	Dibenzothiophene, 4-ethyl-6-methyl
Inchi:	InChI=1S/C15H14S/c1-3-11-7-5-9-13-12-8-4-6-10(2)14(12)16-15(11)13/h4-9H,3H2,1-2H
InchiKey:	INNOFEYMWASFPF-UHFFFAOYSA-N
Formula:	C15H14S
SMILES:	CCc1cccc2c1sc1c(C)cccc12
Mol. weight [g/mol]:	226.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.12		Crippen Method
logp	4.925		Crippen Method
mcvol	180.180	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R86293&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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