

3,7-Dimethyldibenzothiophene

Other names:	Dibenzothiophene, 3,7-dimethyl
Inchi:	InChI=1S/C14H12S/c1-9-3-5-11-12-6-4-10(2)8-14(12)15-13(11)7-9/h3-8H,1-2H3
InchiKey:	ONJGEBKWOANHSB-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	<chem>Cc1ccc2c(c1)sc1cc(C)ccc12</chem>
Mol. weight [g/mol]:	212.31
CAS:	1136-85-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.79		Crippen Method
logp	4.671		Crippen Method
mccvol	166.090	ml/mol	McGowan Method
rinpol	335.80		NIST Webbook
rinpol	334.66		NIST Webbook
rinpol	335.20		NIST Webbook
rinpol	333.38		NIST Webbook
rinpol	336.02		NIST Webbook
rinpol	332.23		NIST Webbook
rinpol	335.10		NIST Webbook
rinpol	335.80		NIST Webbook
rinpol	332.23		NIST Webbook
rinpol	333.38		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=C1136852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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