2,7-Dimethyldibenzothiophene

Other names:	Dibenzothiophene, 3,8-dimethyl
	Dibenzothiophene, 2,7-dimethyl
	3,8-dimethyl-dibenzothiophene
Inchi:	InChI=1S/C14H12S/c1-9-4-6-13-12(7-9)11-5-3-10(2)8-14(11)15-13/h3-8H,1-2H3
InchiKey:	PUENKESSSKIEGY-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	Cc1ccc2c(c1)sc1ccc(C)cc12
Mol. weight [g/mol]:	212.31
CAS:	31317-19-8

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	332.02		NIST Webbook
rinpol	335.33		NIST Webbook
rinpol	336.57		NIST Webbook
rinpol	336.00		NIST Webbook
rinpol	336.10		NIST Webbook
rinpol	333.15		NIST Webbook
rinpol	332.02		NIST Webbook
rinpol	336.09		NIST Webbook
rinpol	336.00		NIST Webbook
rinpol	336.10		NIST Webbook
rinpol	333.15		NIST Webbook
rinpol	336.09		NIST Webbook
rinpol	336.09		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31317198&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