Dibenzothiophene, 4,6-dimethyl-

Other names:	4,6-dimethyldibenzo[b,d]thiophene
	4,6-dimethyldibenzothiophene
Inchi:	InChI=1S/C14H12S/c1-9-5-3-7-11-12-8-4-6-10(2)14(12)15-13(9)11/h3-8H,1-2H3
InchiKey:	MYAQZIAVOLKEGW-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	Cc1cccc2c1sc1c(C)cccc12
Mol. weight [g/mol]:	212.31
CAS:	1207-12-1

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	329.68		NIST Webbook
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
rinpol	328.80		NIST Webbook
rinpol	327.55		NIST Webbook
rinpol	328.32		NIST Webbook
rinpol	329.46		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	329.20		NIST Webbook
rinpol	333.60		NIST Webbook
rinpol	329.17		NIST Webbook
rinpol	327.77		NIST Webbook
rinpol	325.75		NIST Webbook
rinpol	329.17		NIST Webbook
rinpol	329.60		NIST Webbook
rinpol	329.20		NIST Webbook
rinpol	329.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1207121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria for {1-Ethyl-3-methylimidazolium Diethylphosphate or 1-Ethyl-3-methylimidazolium Ethylsulfate} + Alkane Systems:	https://www.doi.org/10.1021/je100991y
Apparent and Partial Molar Volumes at Infinite Dilution and Solid Liquid Equilibrium Data for Dibenzothiophene + 4,6-Dimethyldibenzothiophene + Dodecane Systems at 298.2 K and 313.2 K :	https://www.doi.org/10.1021/je200327s
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

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