

Dibenzothiophene, 3,4-dimethyl

Other names:	3,4-dimethyl-dibenzothiophene
Inchi:	InChI=1S/C14H12S/c1-9-7-8-12-11-5-3-4-6-13(11)15-14(12)10(9)2/h3-8H,1-2H3
InchiKey:	BRZWYUOAWQYIAT-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	<chem>Cc1ccc2c(sc3ccccc32)c1C</chem>
Mol. weight [g/mol]:	212.31

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	336.80		NIST Webbook
rinpol	335.09		NIST Webbook
rinpol	335.10		NIST Webbook
rinpol	334.60		NIST Webbook
rinpol	336.34		NIST Webbook
rinpol	336.34		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R67289&Units=SI
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

Legend

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

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/49-658-8/Dibenzothiophene-3-4-dimethyl.pdf>

Generated by Cheméo on 2024-04-23 16:26:07.346570006 +0000 UTC m=+16178816.267147328.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.