

Dibenzothiophene, 4-ethyl

Other names:	4-ethyl-dibenzothiophene
Inchi:	InChI=1S/C14H12S/c1-2-10-6-5-8-12-11-7-3-4-9-13(11)15-14(10)12/h3-9H,2H2,1H3
InchiKey:	BQANWUIWGKINGF-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	CCc1cccc2c1sc1cccc12
Mol. weight [g/mol]:	212.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	4.617		Crippen Method
mcvol	166.090	ml/mol	McGowan Method
rinpol	326.52		NIST Webbook
rinpol	324.59		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	326.52		NIST Webbook
rinpol	324.59		NIST Webbook
rinpol	2019.00		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=R67328&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

rinpol: Non-polar retention indices

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