

Dibenzothiophene, 2-ethyl

Other names:	2-Ethyldibenzothiophene
Inchi:	InChI=1S/C14H12S/c1-2-10-7-8-14-12(9-10)11-5-3-4-6-13(11)15-14/h3-9H,2H2,1H3
InchiKey:	OIW TUZCEIKRYCP-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	CCc1ccc2sc3ccccc3c2c1
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	328.54		NIST Webbook
rinpol	332.40		NIST Webbook
rinpol	332.50		NIST Webbook
rinpol	332.30		NIST Webbook
rinpol	332.80		NIST Webbook
rinpol	332.65		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=R20950&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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