

Dibenzothiophene, 2-methyl

Other names:	2-Methyldibenzothiophene Dibenzo[b]thiophene, 2-methyl
Inchi:	InChI=1S/C13H10S/c1-9-6-7-13-11(8-9)10-4-2-3-5-12(10)14-13/h2-8H,1H3
InchiKey:	VHUXLBLPAMBOJS-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	<chem>Cc1ccc2sc3ccccc3c2c1</chem>
Mol. weight [g/mol]:	198.28
CAS:	20928-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	4.363		Crippen Method
mcvol	152.000	ml/mol	McGowan Method
rinpol	315.31		NIST Webbook
rinpol	313.83		NIST Webbook
rinpol	313.83		NIST Webbook
rinpol	315.43		NIST Webbook
rinpol	315.20		NIST Webbook
rinpol	315.97		NIST Webbook
rinpol	315.57		NIST Webbook
rinpol	315.70		NIST Webbook
rinpol	316.20		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	315.11		NIST Webbook
rinpol	316.00		NIST Webbook
rinpol	313.71		NIST Webbook
rinpol	314.00		NIST Webbook
rinpol	313.40		NIST Webbook
rinpol	316.00		NIST Webbook
rinpol	314.61		NIST Webbook
rinpol	315.70		NIST Webbook
rinpol	315.80		NIST Webbook
rinpol	316.20		NIST Webbook
rinpol	315.31		NIST Webbook
rinpol	315.20		NIST Webbook
rinpol	315.80		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20928023&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

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