1-Methyldibenzothiophene

Other names:	Dibenzo[b]thiophene, 1-methyl
	Dibenzothiophene, 1-methyl
Inchi:	InChI=1S/C13H10S/c1-9-5-4-8-12-13(9)10-6-2-3-7-11(10)14-12/h2-8H,1H3
InchiKey:	HORCQSAKJDDBKB-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	Cc1cccc2sc3ccccc3c12
Mol. weight [g/mol]:	198.28
CAS:	31317-07-4

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	319.22		NIST Webbook
rinpol	319.22		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	319.60		NIST Webbook
rinpol	319.35		NIST Webbook
rinpol	318.68		NIST Webbook
rinpol	318.65		NIST Webbook
rinpol	310.67		NIST Webbook
rinpol	319.35		NIST Webbook
rinpol	319.75		NIST Webbook
rinpol	318.80		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	319.60		NIST Webbook
rinpol	319.30		NIST Webbook
rinpol	319.69		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	317.10		NIST Webbook
rinpol	320.00		NIST Webbook
rinpol	318.22		NIST Webbook
rinpol	319.20		NIST Webbook
rinpol	319.60		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31317074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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