Dibenzothiophene, 4-methyl-

Other names:	4-methyldibenzo[b,d]thiophene
	4-methyldibenzothiophene
Inchi:	InChI=1S/C13H10S/c1-9-5-4-7-11-10-6-2-3-8-12(10)14-13(9)11/h2-8H,1H3
InchiKey:	NICUQYHIOMMFGV-UHFFFAOYSA-N
Formula:	C13H10S
SMILES:	Cc1cccc2c1sc1ccccc12
Mol. weight [g/mol]:	198.28
CAS:	7372-88-5

Physical Properties

Property code	Value	Unit	Source
hsub	90.30 ± 0.70	kJ/mol	NIST Webbook
log10ws	-5.31		Crippen Method
logp	4.363		Crippen Method
mcvol	152.000	ml/mol	McGowan Method
rinpol	312.22		NIST Webbook
rinpol	311.95		NIST Webbook
rinpol	311.92		NIST Webbook
rinpol	317.78		NIST Webbook
rinpol	312.00		NIST Webbook
rinpol	311.90		NIST Webbook
rinpol	312.73		NIST Webbook
rinpol	312.22		NIST Webbook
rinpol	313.17		NIST Webbook
rinpol	312.40		NIST Webbook
rinpol	312.60		NIST Webbook
rinpol	312.70		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	315.20		NIST Webbook
rinpol	312.72		NIST Webbook
rinpol	311.80		NIST Webbook
rinpol	310.76		NIST Webbook
rinpol	310.90		NIST Webbook
rinpol	310.30		NIST Webbook
rinpol	311.80		NIST Webbook
rinpol	311.34		NIST Webbook
rinpol	312.72		NIST Webbook

rinpol	313.70	NIST Webbook
rinpol	312.50	NIST Webbook
rinpol	312.60	NIST Webbook
rinpol	1927.00	NIST Webbook
rinpol	1927.00	NIST Webbook
rinpol	1932.00	NIST Webbook
rinpol	312.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Apparent and Partial Molar Volumes at Infinite Dilution and Solid Liquid Equilibria of Dibenzothiophene + Alkane Systems:	https://www.doi.org/10.1021/je200327s
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7372885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices