10H-Phenothiazine, 10-methyl-

Other names:	10-Methylphenothiazine
	10-methyl-10H-phenothiazine
	9,10-Dibenzoisothiazine, 10-methyl-
	N-Methylphenothiazine
	Phenothiazide methyl derivative
	Phenothiazine, 10-methyl-
Inchi:	InChI=1S/C13H11NS/c1-14-10-6-2-4-8-12(10)15-13-9-5-3-7-11(13)14/h2-9H,1H3
InchiKey:	QXBUYALKJGBACG-UHFFFAOYSA-N
Formula:	C13H11NS
SMILES:	CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	213.30
CAS:	1207-72-3

Physical Properties

Property code	Value	Unit	Source
ie	6.73 ± 0.07	eV	NIST Webbook
ie	7.15 ± 0.07	eV	NIST Webbook
log10ws	-5.59		Aqueous Solubility Prediction Method
logp	3.919		Crippen Method
mcvol	161.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	103.60	kJ/mol	298.15	Energetic insights on two dye key molecules: N-methylphenothiazine and N-methylphenoxazine

Sources

Energetic insights on two dye key molecules: N-methylphenothiazine and N-methylphenoxazine:	https://www.doi.org/10.1016/j.jct.2015.10.013
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1207723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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