2-Methylphenothiazine

Other names: 10H-Phenothiazine, 2-methyl-
Phenothiazine, 2-methyl-
Inchi: InChI=1S/C13H11NS/c1-9-6-7-13-11(8-9)14-10-4-2-3-5-12(10)15-13/h2-8,14H,1H3
InchiKey: BXXQZMJEARUBHO-UHFFFAOYSA-N
Formula: C13H11NS
SMILES: Cc1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]: 213.30
CAS: 5828-51-3

Physical Properties

Property code	Value	Unit	Source
gf	462.64	kJ/mol	Joback Method
hf	309.37	kJ/mol	Joback Method
hfus	28.75	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.203		Crippen Method
mcvol	161.980	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	668.66	K	Joback Method
tc	939.87	K	Joback Method
tf	540.85	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.94	J/mol×K	668.66	Joback Method
cpg	404.09	J/mol×K	713.86	Joback Method
cpg	417.10	J/mol×K	759.06	Joback Method
cpg	429.08	J/mol×K	804.26	Joback Method
cpg	440.20	J/mol×K	849.46	Joback Method
cpg	450.57	J/mol×K	894.67	Joback Method
cpg	460.36	J/mol×K	939.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5828513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume