2-Methoxyphenothiazine

Other names: 10H-Phenothiazine, 2-methoxy-
2-Methoxy-10H-phenothiazine
Phenothiazine, 2-methoxy-
methyl phenothiazin-2-yl ether
Inchi: InChI=1S/C13H11NOS/c1-15-9-6-7-13-11(8-9)14-10-4-2-3-5-12(10)16-13/h2-8,14H,1H3
InchiKey: DLYKFPHPBCTAKD-UHFFFAOYSA-N
Formula: C13H11NOS
SMILES: COc1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]: 229.30
CAS: 1771-18-2

Physical Properties

Property code	Value	Unit	Source
gf	357.64	kJ/mol	Joback Method
hf	177.15	kJ/mol	Joback Method
hfus	29.94	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.903		Crippen Method
mcvol	167.850	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	691.08	K	Joback Method
tc	957.09	K	Joback Method
tf	563.08	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.86	J/mol×K	691.08	Joback Method
cpg	427.69	J/mol×K	735.41	Joback Method
cpg	440.43	J/mol×K	779.75	Joback Method
cpg	452.19	J/mol×K	824.08	Joback Method
cpg	463.07	J/mol×K	868.42	Joback Method

cpg	473.17	J/mol×K	912.75	Joback Method
cpg	482.60	J/mol×K	957.09	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1771182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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