10H-Phenothiazine, 5-oxide

Other names:	Phenothiazine, 5-oxide
	Phenothiazine S-oxide
	USAF do-16
Inchi:	InChI=1S/C12H9NOS/c14-15-11-7-3-1-5-9(11)13-10-6-2-4-8-12(10)15/h1-8,13H
InchiKey:	DSAFSORWJPSMQS-UHFFFAOYSA-N
Formula:	C12H9NOS
SMILES:	O=S1c2ccccc2Nc2ccccc21
Mol. weight [g/mol]:	215.27
CAS:	1207-71-2

Physical Properties

Property code	Value	Unit	Source
gf	213.02	kJ/mol	Joback Method
hf	93.87	kJ/mol	Joback Method
hfus	30.18	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.910		Crippen Method
mcvol	153.760	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
tb	630.30	K	Joback Method
tc	890.79	K	Joback Method
tf	519.14	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.13	J/mol×K	630.30	Joback Method
cpg	372.85	J/mol×K	673.71	Joback Method
cpg	385.35	J/mol×K	717.13	Joback Method
cpg	396.75	J/mol×K	760.54	Joback Method
cpg	407.18	J/mol×K	803.96	Joback Method
cpg	416.76	J/mol×K	847.37	Joback Method

cpg	425.61	J/mol×K	890.79	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1207712&Units=SI

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