10H-Phenothiazine, 2-chloro-

Other names:	2-chloro-10H-phenothiazine
	2-chlorophenothiazine
	Chlorpromazine M (ring)
	Phenothiazine, 2-chloro-
Inchi:	InChI=1S/C12H8ClNS/c13-8-5-6-12-10(7-8)14-9-3-1-2-4-11(9)15-12/h1-7,14H
InchiKey:	KFZGLJSYQXZIGP-UHFFFAOYSA-N
Formula:	C12H8ClNS
SMILES:	Clc1ccc2c(c1)Nc1ccccc1S2
Mol. weight [g/mol]:	233.72
CAS:	92-39-7

Physical Properties

Property code	Value	Unit	Source
gf	442.29	kJ/mol	Joback Method
hf	314.27	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.548		Crippen Method
mcvol	160.130	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
tb	683.21	K	Joback Method
tc	963.50	K	Joback Method
tf	472.95	K	Solubility determination and thermodynamic functions of 2-chlorophenothiazine in nine organic solvents from T = 283.15 K to T = 318.15 K and mixing properties of solutions
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.10	J/mol×K	683.21	Joback Method
cpg	375.23	J/mol×K	729.93	Joback Method
cpg	386.30	J/mol×K	776.64	Joback Method
cpg	396.47	J/mol×K	823.36	Joback Method
cpg	405.88	J/mol×K	870.07	Joback Method
cpg	414.69	J/mol×K	916.79	Joback Method
cpg	423.05	J/mol×K	963.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility determination and thermodynamic functions of 2-Chlorophenothiazine in nine organic solvents from T = 283.15 K to T = 318.15 K and mixing properties of solutions:	https://www.doi.org/10.1016/j.jct.2016.11.029
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume