

Phenothiazine

Other names:	10H-Phenothiazin
	10H-Phenothiazine
	AFI-Tiazin
	Agrazine
	Antiverm
	Biverm
	Contaverm
	Danikoropa
	Dibenzo-1,4-thiazine
	Dibenzo-p-thiazine
	Dibenzoparathiazine
	Dibenzothiazine
	ENT 38
	EPA Pesticide Chemical Code 064501
	Early bird wormer
	Feeno
	Fenothiazine
	Fenotiazina
	Fenoverm
	Fentiazin
	Helmetina
	Lethelmin
	Nemazene
	Nemazine
	Nexarbol
	Orimon
	Padophene
	Penthazine
	Phenegic
	Phenosan
	Phenoverm
	Phenovis
	Phenoxur
	Phenthiazine
	Phenzeen
	Reconox
	Souframine
	Thiodifenylamine
	Thiodiphenylamin
	Thiodiphenylamine

Property code	Value	Unit	Source
chs	-6777.00 ± 1.60	kJ/mol	NIST Webbook
chs	-6660.09	kJ/mol	NIST Webbook
gf	463.85	kJ/mol	Joback Method
hf	278.20 ± 1.90	kJ/mol	NIST Webbook
hfs	166.70 ± 1.90	kJ/mol	NIST Webbook
hfs	49.71	kJ/mol	NIST Webbook
hfus	26.55	kJ/mol	Joback Method
hsub	111.45 ± 0.37	kJ/mol	NIST Webbook
hsub	114.50 ± 0.40	kJ/mol	NIST Webbook
hvap	60.80	kJ/mol	Joback Method
ie	6.74 ± 0.07	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	6.96 ± 0.19	eV	NIST Webbook
ie	6.87	eV	NIST Webbook
ie	7.62	eV	NIST Webbook
ie	7.26 ± 0.08	eV	NIST Webbook
log10ws	-5.26		Aqueous Solubility Prediction Method
logp	3.895		Crippen Method
mcvol	147.890	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2010.00		NIST Webbook

rinpol	2010.00		NIST Webbook
tb	644.20	K	NIST Webbook
tc	918.16	K	Joback Method
tf	457.55 ± 0.40	K	NIST Webbook
tf	458.50 ± 0.20	K	NIST Webbook
tf	457.50 ± 0.20	K	NIST Webbook
tf	458.39 ± 0.20	K	NIST Webbook
tf	456.00	K	Solubility of Phenothiazine in Water, Ethanol, and Propylene Glycol at (298.2 to 338.2) K and Their Binary and Ternary Mixtures at 298.2 K
tf	457.90	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements
tf	458.85	K	Structural, energetic and reactivity properties of phenoxazine and phenothiazine
tf	458.90	K	Aqueous Solubility Prediction Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.13	J/molxK	918.16	Joback Method
cpg	356.29	J/molxK	687.03	Joback Method
cpg	368.70	J/molxK	733.25	Joback Method
cpg	380.03	J/molxK	779.48	Joback Method
cpg	390.44	J/molxK	825.71	Joback Method
cpg	400.08	J/molxK	871.93	Joback Method
cpg	342.65	J/molxK	640.80	Joback Method
hfust	25.66	kJ/mol	458.40	NIST Webbook
hfust	28.40	kJ/mol	457.20	NIST Webbook
hfust	25.70	kJ/mol	458.40	NIST Webbook
hfust	26.92	kJ/mol	458.20	NIST Webbook
hfust	26.92	kJ/mol	458.20	NIST Webbook
hsubt	86.00	kJ/mol	365.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.06683e+01
Coeff. B	-1.03386e+04
Temperature range (K), min.	507.27
Temperature range (K), max.	673.22

Sources

Solubility of Phenothiazine in Water, Ethanol, and Propylene Glycol at (298.2 to 362.2 K) and Their Binary and Ternary Mixtures at 298.2 K: McGowan Method:	https://www.doi.org/10.1021/je2001649
	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92842&Units=SI
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Structural, energetic and reactivity properties of phenoxazine and phenothiazine:	https://www.doi.org/10.1016/j.jct.2013.11.013
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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