

Phenoxazine

Other names:	10H-Phenoxazine 2,3:5,6-Dibenzo-1,4-oxazine NSC 72990 Phenazoxine
Inchi:	InChI=1S/C12H9NO/c1-3-7-11-9(5-1)13-10-6-2-4-8-12(10)14-11/h1-8,13H
InchiKey:	TZMSYXZUNZXBOL-UHFFFAOYSA-N
Formula:	C12H9NO
SMILES:	<chem>c1ccc2c(c1)Nc1cccc1O2</chem>
Mol. weight [g/mol]:	183.21
CAS:	135-67-1

Physical Properties

Property code	Value	Unit	Source
chs	-6006.30 ± 2.70	kJ/mol	NIST Webbook
gf	337.87	kJ/mol	Joback Method
hf	94.00 ± 2.80	kJ/mol	NIST Webbook
hfs	-2.10 ± 2.80	kJ/mol	NIST Webbook
hfus	30.87	kJ/mol	Joback Method
hsub	96.08 ± 0.31	kJ/mol	NIST Webbook
hsub	96.10 ± 0.30	kJ/mol	NIST Webbook
hvap	59.50	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.536		Crippen Method
mcvol	137.410	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	619.92	K	Joback Method
tc	881.44	K	Joback Method
tf	429.85 ± 0.50	K	NIST Webbook
tf	430.73	K	Structural, energetic and reactivity properties of phenoxazine and phenothiazine
vc	0.515	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.11	J/molxK	619.92	Joback Method
cpg	342.71	J/molxK	663.51	Joback Method
cpg	355.12	J/molxK	707.09	Joback Method
cpg	366.49	J/molxK	750.68	Joback Method
cpg	376.92	J/molxK	794.27	Joback Method
cpg	386.54	J/molxK	837.85	Joback Method
cpg	395.48	J/molxK	881.44	Joback Method
psub	1.02e-04	kPa	340.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	5.94e-05	kPa	336.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.02e-04	kPa	340.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	2.81e-05	kPa	329.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

psub	1.64e-04	kPa	344.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.64e-04	kPa	345.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.96e-04	kPa	346.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	2.20e-04	kPa	348.20	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	3.45e-04	kPa	352.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

psub	3.63e-04	kPa	353.10	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	4.83e-04	kPa	356.70	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	7.48e-04	kPa	360.90	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique
psub	1.07e-03	kPa	364.50	Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique: *Journal of Chemical Thermodynamics*

<https://www.doi.org/10.1016/j.jct.2010.01.014>

<https://www.doi.org/10.1016/j.jct.2013.11.013>

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=C135671&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
hsub:	Enthalpy of sublimation 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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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