Antazoline

Other names:	1H-Imidazole-2-methanamine, 4,5-dihydro-N-phenyl-N-(phenylmethyl)-
	2-(N-Phenyl-N-benzylaminomethyl)imidazoline
	2-Imidazoline, 2-[(N-benzylanilino)methyl]-
	2-Phenyl-benzyl-amino-methylimidazolin
	2-[(N-Benzylanilino)methyl]-2-imidazoline
	4,5-Dihydro-N-phenyl-N-phenylmethyl-1H-imidazole-2-methanamine
	5512-M
	Allergan A
	Analergine
	Antastan
	Antasten
	Antazolin
	Antihistal
	Antistin
	Antistine
	Azalone
	Ben-a-hist
	Histostab
	Imidamine
	Phenazoline
Inchi:	InChI=1S/C17H19N3/c1-3-7-15(8-4-1)13-20(14-17-18-11-12-19-17)16-9-5-2-6-10-16/h1-
InchiKey:	REYFJDPCWQRWAA-UHFFFAOYSA-N
Formula:	C17H19N3
SMILES:	c1ccc(CN(CC2=NCCN2)c2ccccc2)cc1
Mol. weight [g/mol]:	265.35
CAS:	91-75-8

Physical Properties

Property code	Value	Unit	Source
gf	696.94	kJ/mol	Joback Method
hf	382.29	kJ/mol	Joback Method
hfus	39.31	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-2.60		Aqueous Solubility Prediction Method
logp	2.695		Crippen Method
mcvol	217.650	ml/mol	McGowan Method

pc	2684.64	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2328.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	780.50	K	Joback Method
tc	1042.79	K	Joback Method
tf	571.65	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.54	J/mol×K	780.50	Joback Method
cpg	668.03	J/mol×K	824.21	Joback Method
cpg	684.73	J/mol×K	867.93	Joback Method
cpg	699.76	J/mol×K	911.64	Joback Method
cpg	713.24	J/mol×K	955.36	Joback Method
cpg	725.27	J/mol×K	999.07	Joback Method
cpg	735.98	J/mol×K	1042.79	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91758&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume