Phenylethanolamine

Other names:	(.+/-.)-Phenylethanolamine
	(RS)-2-Amino-1-phenylethanol
	2-Amino-1-phenyl-1-ethanol
	2-Amino-1-phenylethanol
	2-Hydroxy-2-phenylethylamine
	2-Phenyl-2-hydroxyethylamine
	Benzeneethanamine, «beta»-hydroxy-
	Benzeneethanamine, Â«betaÂ»-hydroxy-
	Benzenemethanol, «alpha»-(aminomethyl)-
	Benzenemethanol, Â«alphaÂ»-(aminomethyl)-
	Benzyl alcohol, «alpha»-(aminomethyl)-
	Benzyl alcohol, Â«alphaÂ»-(aminomethyl)-
	Bisnorephedrine
	Ethanol, 2-amino-1-phenyl-
	Ethylamine, «beta»-hydroxy-«beta»-phenyl-
	Ethylamine, Â«betaÂ»-hydroxy-Â«betaÂ»-phenyl-
	NSC 46837
	NSC 5021
	Phenethanolamine
	Phenethylamine, «beta»-hydroxy-
	Phenethylamine, Â«betaÂ»-hydroxy-
	dl-«beta»-Phenyl-«beta»-hydroxyethylamine
	dl-Â«betaÂ»-Phenyl-Â«betaÂ»-hydroxyethylamine
	«alpha»-(Aminomethyl)benzyl alcohol
	«beta»-Hydroxy-«beta»-phenylethylamine
	«beta»-Hydroxyphenethylamine
	«beta»-Hydroxyphenylethylamine
	«beta»-Phenethanolamine
	«beta»-Phenylethanolamine
	Â«alphaÂ»-(Aminomethyl)benzyl alcohol
	Â«betaÂ»-Hydroxy-Â«betaÂ»-phenylethylamine
	Â«betaÂ»-Hydroxyphenethylamine
	Â«betaÂ»-Hydroxyphenylethylamine
	Â«betaÂ»-Phenethanolamine
	Â«betaÂ»-Phenylethanolamine
Inchi:	InChI=1S/C8H11NO/c9-6-8(10)7-4-2-1-3-5-7/h1-5,8,10H,6,9H2
InchiKey:	ULSIYEODSMZIPX-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	NCC(O)c1ccccc1
Mol. weight [g/mol]:	137.18

CAS: 7568-93-6

Physical Properties

Property code	Value	Unit	Source
gf	56.08	kJ/mol	Joback Method
hf	-95.64	kJ/mol	Joback Method
hfus	16.28	kJ/mol	Joback Method
hvap	62.61	kJ/mol	Joback Method
log10ws	-0.48		Aqueous Solubility Prediction Method
logp	0.679		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	573.39	K	Joback Method
tc	784.75	K	Joback Method
tf	329.90	K	Aqueous Solubility Prediction Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.53	J/mol×K	573.39	Joback Method
cpg	287.40	J/mol×K	608.62	Joback Method
cpg	297.57	J/mol×K	643.84	Joback Method
cpg	307.08	J/mol×K	679.07	Joback Method
cpg	315.94	J/mol×K	714.30	Joback Method
cpg	324.21	J/mol×K	749.52	Joback Method
cpg	331.92	J/mol×K	784.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	2.30	NIST Webbook

Sources

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=C7568936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume