Phenol, 4-(2-aminoethyl)-

Other names:	2-(4'-Hydroxyphenyl)ethylamine
	2-(4-Hydroxyphenyl)ethylamine
	2-(p-Hydroxyphenyl)ethylamine
	4-(2-Aminoethyl)phenol
	4-Hydroxy-«beta»-phenylethylamine
	4-Hydroxy-Â«betaÂ»-phenylethylamine
	4-Hydroxyphenethylamine
	4-Hydroxyphenylethylamine
	Benzeneethanamine, 4-hydroxy-
	NSC 249188
	Phenethylamine, p-hydroxy-
	Phenol, p-(2-aminoethyl)-
	Systogene
	Tenosin-Wirkstoff
	Tocosine
	Tyramin
	Tyramine
	Tyramine base
	Tyrosamine
	Uteramine
	p-(2-Aminoethyl)phenol
	p-Hydroxy-«beta»-phenethylamine
	p-Hydroxy-«beta»-phenylethylamine
	p-Hydroxy-Â«betaÂ»-phenethylamine
	p-Hydroxy-Â«betaÂ»-phenylethylamine
	p-Hydroxyphenethylamine
	p-Hydroxyphenylethylamine
	p-Tyramine
	p-«beta»-Aminoethylphenol
	p-Â«betaÂ»-Aminoethylphenol
	«alpha»-(4-Hydroxyphenyl)-«beta»-aminoethane
	«beta»-(4-Hydroxyphenyl)ethylamine
	Â«alphaÂ»-(4-Hydroxyphenyl)-Â«betaÂ»-aminoethane
	Â«betaÂ»-(4-Hydroxyphenyl)ethylamine
Inchi:	InChI=1S/C8H11NO/c9-6-5-7-1-3-8(10)4-2-7/h1-4,10H,5-6,9H2
InchiKey:	DZGWFCGJZKJUFP-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	NCCc1ccc(O)cc1
Mol. weight [g/mol]:	137.18
CAS:	51-67-2

Physical Properties

Property code	Value	Unit	Source
gf	40.72	kJ/mol	Joback Method
hf	-115.44	kJ/mol	Joback Method
hfus	21.50	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
ie	8.41 ± 0.12	eV	NIST Webbook
log10ws	-1.12		Aqueous Solubility Prediction Method
logp	0.893		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1660.90		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1660.90		NIST Webbook
tb	562.27	K	Joback Method
tc	798.02	K	Joback Method
tf	437.32	K	Aqueous Solubility Prediction Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.50	J/mol×K	562.27	Joback Method
cpg	288.09	J/mol×K	601.56	Joback Method
cpg	298.81	J/mol×K	640.85	Joback Method
cpg	308.74	J/mol×K	680.15	Joback Method
cpg	317.98	J/mol×K	719.44	Joback Method
cpg	326.61	J/mol×K	758.73	Joback Method
cpg	334.74	J/mol×K	798.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.20	K	1.00	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=C51672&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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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