Phenylephrine

Other names:
(-)-Phenylephrine
(-)-m-Hydroxy-«alpha»-(methylaminomethyl)benzyl alcohol
(-)-m-Hydroxy-Â«alphaÂ»-(methylaminomethyl)benzyl alcohol
(-)-m-Oxedrine
(R)-3-Hydroxy-«alpha»-[(methylamino)methyl]benzenemethanol
(R)-3-Hydroxy-Â«alphaÂ»-[(methylamino)methyl]benzenemethanol
3-[1-Hydroxy-2-(methylamino)ethyl]phenol, (R)-
Benzenemethanol, 3-hydroxy-a-[(methylamino)methyl]-, («alpha»R)-
Benzenemethanol, 3-hydroxy-a-[(methylamino)methyl]-, (Â«alphaÂ»R)-
Benzenemethanol, 3-hydroxy-«alpha»-[(methylamino)methyl]-, (R)-
Benzenemethanol, 3-hydroxy-Â«alphaÂ»-[(methylamino)methyl]-, (R)-
Benzyl alcohol, m-hydroxy-«alpha»-((methylamino)methyl)-, (-)-
Benzyl alcohol, m-hydroxy-Â«alphaÂ»-((methylamino)methyl)-, (-)-
Isophrin
Mesaton
Mesatone
Metaoxedrin
Metaoxedrine
Metasympatol
Metasynephrine
Mezaton
Neosynephrine
R(-)-Mezaton
R(-)-Phenylephrine
Visadron
l-(3-Hydroxyphenyl)-N-methylethanolamine
l-1-(m-Hydroxyphenyl)-2-methylaminoethanol
l-m-Hydroxy-«alpha»-((methylamino)methyl)benzyl alcohol
l-m-Hydroxy-Â«alphaÂ»-((methylamino)methyl)benzyl alcohol
l-«alpha»-Hydroxy-«beta»-methylamino-3-hydroxy-l-ethylbenzene
l-Â«alphaÂ»-Hydroxy-Â«betaÂ»-methylamino-3-hydroxy-l-ethylbenzene
m-Methylaminoethanolphenol
m-Oxedrine
m-Sympathol
m-Sympatol
m-Synephrine

Inchi: InChI=1S/C9H13NO2/c1-10-6-9(12)7-3-2-4-8(11)5-7/h2-5,9-12H,6H2,1H3/t9-/m1/s1

InchiKey: SONNWYBIRXJNDC-SECBINFHSA-N

Formula: C9H13NO2

SMILES: CNCC(O)c1cccc(O)c1

Mol. weight [g/mol]: 167.21
CAS: 59-42-7

Physical Properties

Property code	Value	Unit	Source
gf	-67.18	kJ/mol	Joback Method
hf	-273.91	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	0.58		Aqueous Solubility Prediction Method
logp	0.645		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	4510.35	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	654.53	K	Joback Method
tc	864.38	K	Joback Method
tf	415.65	K	Aqueous Solubility Prediction Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.90	J/mol×K	654.53	Joback Method
cpg	371.37	J/mol×K	689.51	Joback Method
cpg	381.18	J/mol×K	724.48	Joback Method
cpg	390.40	J/mol×K	759.46	Joback Method
cpg	399.12	J/mol×K	794.43	Joback Method
cpg	407.38	J/mol×K	829.41	Joback Method
cpg	415.28	J/mol×K	864.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59427&Units=SI
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

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