

Octopamine

Other names:	Benzenemethanol, «alpha»-(aminomethyl)-4-hydroxy- Benzyl alcohol, «alpha»-(aminomethyl)-p-hydroxy- «alpha»-(Aminomethyl)-p-hydroxybenzyl alcohol 1-(p-Hydroxyphenyl)-2-aminoethanol p-Hydroxyphenylethanolamine Norden Norphen Norsympathol Norsynephrine Paraoxyphenyl aminoethanol WIN 5512 dl-Octopamine (. +/-.)-«alpha»-(Aminomethyl)-p-hydroxybenzyl alcohol ND 50 Norsympatol (. +/-.)-Octopamine Analet
Inchi:	InChI=1S/C8H11NO2/c9-5-8(11)6-1-3-7(10)4-2-6/h1-4,8,10-11H,5,9H2
InchiKey:	QHGUCRYDKWKLMG-UHFFFAOYSA-N
Formula:	C8H11NO2
SMILES:	NCC(O)c1ccc(O)cc1
Mol. weight [g/mol]:	153.18
CAS:	104-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-98.54	kJ/mol	Joback Method
hf	-272.95	kJ/mol	Joback Method
hfus	22.06	kJ/mol	Joback Method
hvap	75.62	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.384		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	654.01	K	Joback Method
tc	875.02	K	Joback Method
tf	447.14	K	Joback Method

vc	0.384	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.15	J/mol×K	654.01	Joback Method
cpg	329.53	J/mol×K	690.84	Joback Method
cpg	338.27	J/mol×K	727.68	Joback Method
cpg	346.47	J/mol×K	764.51	Joback Method
cpg	354.20	J/mol×K	801.35	Joback Method
cpg	361.53	J/mol×K	838.18	Joback Method
cpg	368.56	J/mol×K	875.02	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C104143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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