Benzenemethanol, 4-hydroxy-«alpha»-[1-(methylamino)ethyl]-, (R*,S*)-

Other names:	Benzyl alcohol, p-hydroxy-«alpha»-(1-(methylamino)ethyl)-
	Hydroxyephedrine
	p-Hydroxyephedrine
	4-Hydroxyephedrine
	Methylsympatol
	p-Oxy-ephedrin
	Oxyephedrine
	Suprifen
	Suprifene
	Supriphen
	Ephedrine, p-hydroxy-
	Oxilofrine
	(R*,S*)-4-hydroxy-«alpha»-[1-(methylamino)ethyl]benzyl alcohol
Inchi:	InChI=1S/C10H15NO2/c1-7(11-2)10(13)8-3-5-9(12)6-4-8/h3-7,10-13H,1-2H3
InchiKey:	OXFGTKPPFSCSMA-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	CNC(C)C(O)c1ccc(O)cc1
Mol. weight [g/mol]:	181.23
CAS:	365-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-61.20	kJ/mol	Joback Method
hf	-299.83	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.033		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook
tb	676.97	K	Joback Method
tc	887.54	K	Joback Method
tf	424.08	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.56	J/mol×K	676.97	Joback Method
cpg	421.95	J/mol×K	712.06	Joback Method
cpg	432.64	J/mol×K	747.16	Joback Method
cpg	442.70	J/mol×K	782.25	Joback Method
cpg	452.22	J/mol×K	817.35	Joback Method
cpg	461.26	J/mol×K	852.44	Joback Method
cpg	469.91	J/mol×K	887.54	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C365264&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume