Nylidrin

Other names:	Benzenemethanol, 4-hydroxy-«alpha»-[1-[(1-methyl-3-phenylpropyl)amino]ethyl]-
	Benzyl alcohol, p-hydroxy-«alpha»-[1-[(1-methyl-3-phenylpropyl)amino]ethyl]-
	Buphenin
	Buphenine
	Nilidrine
	Phenyl-sec-butyl norsuprifen
	Suprifen-psb
	p-Hydroxy-«alpha»-[1-[(methyl-3-phenylpropyl)amino]ethyl]benzyl alcohol
	1-(p-Hydroxyphenyl)-2-(1'-methyl-3'-phenylpropylamino)-1-propanol
	p-Hydroxy-N-(1-methyl-3-phenylpropyl)norephedrine
Inchi:	InChI=1S/C19H25NO2/c1-14(8-9-16-6-4-3-5-7-16)20-15(2)19(22)17-10-12-18(21)13-11-
InchiKey:	PTGXAUBQBSGPKF-UHFFFAOYSA-N
Formula:	C19H25NO2
SMILES:	CC(CCc1ccccc1)NC(C)C(O)c1ccc(O)cc1
Mol. weight [g/mol]:	299.41
CAS:	447-41-6

Physical Properties

Property code	Value	Unit	Source
gf	124.55	kJ/mol	Joback Method
hf	-254.34	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	97.40	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.425		Crippen Method
mcvol	252.770	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	909.13	K	Joback Method
tc	1134.03	K	Joback Method
tf	536.93	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.39	J/mol×K	909.13	Joback Method
cpg	822.75	J/mol×K	946.61	Joback Method
cpg	836.45	J/mol×K	984.10	Joback Method
cpg	849.64	J/mol×K	1021.58	Joback Method
cpg	862.44	J/mol×K	1059.07	Joback Method
cpg	875.00	J/mol×K	1096.55	Joback Method
cpg	887.43	J/mol×K	1134.03	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C447416&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