Alprenolol

Other names:	(±) 1-(o-allylphenoxy)-3-(isopropylamino)-2-propanol (alprenolol)
	(Â±) 1-(o-allylphenoxy)-3-(isopropylamino)-2-propanol (alprenolol)
	1-(o-Allylphenoxy)-3-(isopropylamino)-2-propanol
	1-(propan-2-ylamino)-3-(2-prop-2-enylphenoxy)propan-2-ol
	2-Propanol, 1-(o-allylphenoxy)-3-(isopropylamino)-
	2-Propanol, 1-[(1-methylethyl)amino]-3-[2-(2-propenyl)phenoxy]-
	Alfeprol
	Alpheprol
	H 56/28
Inchi:	InChI=1S/C15H23NO2/c1-4-7-13-8-5-6-9-15(13)18-11-14(17)10-16-12(2)3/h4-6,8-9,12,1
InchiKey:	PAZJSJFMUHDSTF-UHFFFAOYSA-N
Formula:	C15H23NO2
SMILES:	C=CCc1ccccc1OCC(O)CNC(C)C
Mol. weight [g/mol]:	249.35
CAS:	13655-52-2

Physical Properties

Property code	Value	Unit	Source
gf	108.73	kJ/mol	Joback Method
hf	-243.98	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-1.78		Aqueous Solubility Prediction Method
logp	2.153		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	734.83	K	Joback Method
tc	928.30	K	Joback Method
tf	381.48	K	Aqueous Solubility Prediction Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.59	J/mol×K	896.05	Joback Method
cpg	622.12	J/mol×K	734.83	Joback Method
cpg	636.66	J/mol×K	767.07	Joback Method
cpg	650.34	J/mol×K	799.32	Joback Method
cpg	663.20	J/mol×K	831.56	Joback Method
cpg	675.28	J/mol×K	863.81	Joback Method
cpg	697.18	J/mol×K	928.30	Joback Method
hfust	35.61	kJ/mol	331.20	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13655522&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

hfust: Enthalpy of fusion at a given temperature

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