Nadolol

Other names:	1-(tert-Butylamino)-3-((5,6,7,8-tetrahydro-cis-6,7-dihydroxy-1-naphthyl)oxy)-2-propanol
	2,3-Naphthalenediol, 5-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]-1,2,3,4-tetrahydro-
	2,3-Naphthalenediol, 5-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]-1,2,3,4-tetrahydro-, cis-
	2,3-cis-1,2,3,4-Tetrahydro-5-((2-hydroxy-3-tert-butylamino)propoxy)-2,3-naphthalenediol
	5-(3-((1,1-Dimethylethyl)amino)-2-hydroxypropoxy)-1,2,3,4-tetrahydro-2,3-naphthalenedio
	5-(3-(tert-butylamino)-2-hydroxypropoxy)-1,2,3,4-tetrahydronaphthalene-2,3-diol
	5-[3-(tert-Butylamino)-2-hydroxypropoxy]-1,2,3,4-tetrahydro-2,3-naphthalenediol, cis-
	Anabet
	Corgard
	SQ 11725
	Solgol
Inchi:	InChI=1S/C17H27NO4/c1-17(2,3)18-9-12(19)10-22-16-6-4-5-11-7-14(20)15(21)8-13(11)1
InchiKey:	VWPOSFSPZNDTMJ-UHFFFAOYSA-N
Formula:	C17H27NO4
SMILES:	CC(C)(C)NCC(O)COc1cccc2c1CC(O)C(O)C2
Mol. weight [g/mol]:	309.40
CAS:	42200-33-9

Physical Properties

Property code	Value	Unit	Source
gf	-199.32	kJ/mol	Joback Method
hf	-683.79	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	114.01	kJ/mol	Joback Method
log10ws	-1.01		Aqueous Solubility Prediction Method
logp	0.635		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	2633.00		NIST Webbook
tb	976.80	K	Joback Method
tc	1195.88	K	Joback Method
tf	403.40	K	Solubility and pKa of select pharmaceuticals in water, ethanol, and 1-octanol
tf	400.65	K	Aqueous Solubility Prediction Method

vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.39	J/mol×K	976.80	Joback Method
cpg	877.76	J/mol×K	1013.31	Joback Method
cpg	889.28	J/mol×K	1049.83	Joback Method
cpg	900.04	J/mol×K	1086.34	Joback Method
cpg	910.10	J/mol×K	1122.85	Joback Method
cpg	919.56	J/mol×K	1159.37	Joback Method
cpg	928.48	J/mol×K	1195.88	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42200339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility and pKa of select pharmaceuticals in water, ethanol, and 1-octanol:	https://www.doi.org/10.1016/j.jct.2010.07.001
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