Labetalol

Other names:	2-Hydroxy-5-(1-hydroxy-2-[(1-methyl-3-phenylpropyl)amino]ethyl)benzamide
	3-Carboxamido-4-hydroxy-«alpha»-((1-methyl-3-phenylpropylamino)methyl)benzyl alcohol
	5-(1-Hydroxy-2-(1-methyl-3-phenylpropylamino)ethyl)salicylamide
	AH 5158
	Albetol
	Benzamide, 2-hydroxy-5-[1-hydroxy-2-[(1-methyl-3-phenylpropyl)amino]ethyl]-
	Ibidomide
	ScH 15719W
Inchi:	InChI=1S/C19H24N2O3/c1-13(7-8-14-5-3-2-4-6-14)21-12-18(23)15-9-10-17(22)16(11-15
InchiKey:	SGUAFYQXFOLMHL-UHFFFAOYSA-N
Formula:	C19H24N2O3
SMILES:	CC(CCc1ccccc1)NCC(O)c1ccc(O)c(C(N)=O)c1
Mol. weight [g/mol]:	328.41
CAS:	36894-69-6

Physical Properties

Property code	Value	Unit	Source
gf	54.89	kJ/mol	Joback Method
hf	-339.32	kJ/mol	Joback Method
hfus	47.38	kJ/mol	Joback Method
hvap	115.84	kJ/mol	Joback Method
log10ws	-1.30		Aqueous Solubility Prediction Method
logp	2.135		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
tb	1040.95	K	Joback Method
tc	1281.29	K	Joback Method
tf	463.65	K	Aqueous Solubility Prediction Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	877.35	J/mol×K	1040.95	Joback Method
cpg	890.44	J/mol×K	1081.01	Joback Method
cpg	903.25	J/mol×K	1121.06	Joback Method
cpg	915.91	J/mol×K	1161.12	Joback Method
cpg	928.60	J/mol×K	1201.18	Joback Method
cpg	941.46	J/mol×K	1241.23	Joback Method
cpg	954.64	J/mol×K	1281.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36894696&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

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