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

Physical Properties

Property code	Value	Unit	Source
hfus	47.38	kJ/mol	Joback Method
log10ws	-1.30		Aqueous Solubility Prediction Method
logp	2.135		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
tf	463.65	K	Aqueous Solubility Prediction 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

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36894696&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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