Acebutolol

Other names: (.+/-.)-3'-Acetyl-4'-[2-hydroxy-3-(1-methylethylamino)propoxy]butyranilide
(.+/-.)-3'-Acetyl-4'-[2-hydroxy-3-(isopropylamino)propoxy]butyranilide
(.+/-.)-Acebutolol
(.+/-.)-N-(3-Acetyl-4-(2-hydroxy-3-((1-methylethyl)amino)propoxy)phenyl)butanamide
1-(2-Acetyl-4-n-butyramidophenoxy)-2-hydroxy-3-isopropylaminopropane
3'-Acetyl-4'-(2-hydroxy-3-(isopropylamino)propoxy)butyranilide
5'-Butyramido-2'-(2-hydroxy-3-isopropylaminopropoxy)acetophenone
Butanamide, N-[3-acetyl-4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]phenyl]-
Butanamide, N-[3-acetyl-4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]phenyl]-, (.+/-.)-
Monitan
Neptal
Prent
dl-Acebutolol

Inchi: InChI=1S/C18H28N2O4/c1-5-6-18(23)20-14-7-8-17(16(9-14)13(4)21)24-11-15(22)10-19-

InchiKey: GOEMGAFJFRBGGG-UHFFFAOYSA-N

Formula: C18H28N2O4

SMILES: CCCC(=O)Nc1ccc(OCC(O)CNC(C)C)c(C(C)=O)c1

Mol. weight [g/mol]: 336.43

CAS: 37517-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-131.93	kJ/mol	Joback Method
hf	-614.49	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	103.94	kJ/mol	Joback Method
log10ws	-2.71		Aqueous Solubility Prediction Method
logp	2.365		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		NIST Webbook
tb	969.68	K	Joback Method
tc	1188.02	K	Joback Method
tf	393.75	K	Aqueous Solubility Prediction Method

vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.15	J/mol×K	969.68	Joback Method
cpg	915.38	J/mol×K	1006.07	Joback Method
cpg	926.48	J/mol×K	1042.46	Joback Method
cpg	936.48	J/mol×K	1078.85	Joback Method
cpg	945.43	J/mol×K	1115.24	Joback Method
cpg	953.35	J/mol×K	1151.63	Joback Method
cpg	960.30	J/mol×K	1188.02	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37517309&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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