Atenolol

Other names:

(+) 4-[2'-Hydroxy-3'-(isopropylamino)propoxy]-phenylacetamide (atenolol)
1-p-Carbamoylmethylphenoxy-3-isopropylamino-2-propanol
2-(4-[2-Hydroxy-3-(isopropylamino)propoxy]phenyl)acetamide
2-(p-(2-Hydroxy-3-(isopropylamino)propoxy)phenyl)acetamide
4-(2-Hydroxy-3-((1-methylethyl)amino)propoxy)benzeneacetamide
Acetamide, 2-(p-(2-hydroxy-3-(isopropylamino)propoxy)phenyl)-
Alinor
Altol
Anselol
Antipressan
Apo-Atenolol
Atcardil
Atecard
Atehexal
Atenblock
Atendol
Atenet
Ateni
Atenil
Atenol
Atereal
Aterol
Benzeneacetamide, 4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-
Betablok
Betacard
Blokium
Corotenol
Cuxanorm
Duraatenolol
Evitocor
Farnormin
Felo-Bits
Hipres
Hypoten
ICI 66082
Ibinolo
Internolol
Lo-ten
Lotenal
Myocord

Normalol
Normiten
Noten
Oraday
Premorine
Prenolol
Prenormine
Seles beta
Selobloc
Serten
Stermin
Tenidon
Teno-basan
Tenoblock
Tenolol
Tenoprin
Tenormin
Tenormine
Tensimin
Tredol
Uniloc
Vascoten
Vericordin
Wesipin
Xaten

Inchi: InChI=1S/C14H22N2O3/c1-10(2)16-8-12(17)9-19-13-5-3-11(4-6-13)7-14(15)18/h3-6,10,1

InchiKey: METKIMKYRPQLGS-UHFFFAOYSA-N

Formula: C14H22N2O3

SMILES: CC(C)NCC(O)COc1ccc(CC(N)=O)cc1

Mol. weight [g/mol]: 266.34

CAS: 29122-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-50.00	kJ/mol	Joback Method
hf	-427.56	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hsub	140.00 ± 3.70	kJ/mol	NIST Webbook
hvap	91.83	kJ/mol	Joback Method

log10ws	0.04		Aqueous Solubility Prediction Method
logp	0.452		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
tb	841.67	K	Joback Method
tc	1049.15	K	Joback Method
tf	419.75	K	Aqueous Solubility Prediction Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.19	J/mol×K	841.67	Joback Method
cpg	683.46	J/mol×K	876.25	Joback Method
cpg	694.83	J/mol×K	910.83	Joback Method
cpg	705.32	J/mol×K	945.41	Joback Method
cpg	714.96	J/mol×K	979.99	Joback Method
cpg	723.79	J/mol×K	1014.57	Joback Method
cpg	731.83	J/mol×K	1049.15	Joback Method
hfust	38.70	kJ/mol	426.10	NIST Webbook
hfust	35.66	kJ/mol	423.40	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29122687&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsub:	Enthalpy of sublimation 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