Isoproterenol

Other names:

(.+/-.)-Isoprenaline
(.+/-.)-Isoproterenol
1,2-Benzenediol, 4-[1-hydroxy-2-[(1-methylethyl)amino]ethyl]-
1-(3,4-Dihydroxyphenyl)-2-(isopropylamino)ethanol
3,4-Dihydroxy-«alpha»-(isopropylaminomethyl)-benzyl alcohol
3,4-Dihydroxy-Â«alphaÂ»-(isopropylaminomethyl)-benzyl alcohol
4-(1-Hydroxy-2-((1-methylethyl)amino)ethyl)-1,2-benzenediol
A 21
Aleudrine
Aludrin
Aludrine
Asiprenol
Asmalar
Assiprenol
Bellasthman
Benzyl alcohol, 3,4-dihydroxy-«alpha»-((isopropylamino)methyl)-
Benzyl alcohol, 3,4-dihydroxy-Â«alphaÂ»-((isopropylamino)methyl)-
Bronkephrine
DL(.+/-.)-Isoproterenol
Dihydroxyphenylethanolisopropylamine
Epinephrine isopropyl homolog
ICI 46399
Isadrine
Isonorene
Isonorin
Isoprenalin
Isoprenaline
Isopropydrin
Isopropyladrenaline
Isopropylaminomethyl(3,4-dihydroxyphenyl)carbinol
Isopropylarterenol
Isopropylnoradrenaline
Isopropylnorepinephrine
Isorenin
Isupren
Lomupren
N-Isopropyl-«beta»-dihydroxyphenyl-«beta»-hydroxyethylamine
N-Isopropyl-Â«betaÂ»-dihydroxyphenyl-Â«betaÂ»-hydroxyethylamine
N-Isopropylnoradrenaline
N-Isopropylnorepinephrine

Neodrenal
Norisodrine
Novodrin
Proternol
Protocatechuyl alcohol,«alpha»-(isopropylamino-methyl),-
Protocatechuyl alcohol,Â«alphaÂ»-(isopropylamino-methyl),-
Racemic isoprenaline
Racemic isoproterenol
Respifral
Saventrine
Vapo-N-iso
WIN 5162
dl-Isadrine
neo-Epinine
«alpha»-(Isopropylaminomethyl)protocatechuyl alcohol
«alpha»-(Isopropylaminomoethyl)protocatechuyl alcohol
Â«alphaÂ»-(Isopropylaminomethyl)protocatechuyl alcohol
Â«alphaÂ»-(Isopropylaminomoethyl)protocatechuyl alcohol

Inchi: InChI=1S/C11H17NO3/c1-7(2)12-6-11(15)8-3-4-9(13)10(14)5-8/h3-5,7,11-15H,6H2,1-2H

InchiKey: JWZZKOKVBUJMES-UHFFFAOYSA-N

Formula: C11H17NO3

SMILES: CC(C)NCC(O)c1ccc(O)c(O)c1

Mol. weight [g/mol]: 211.26

CAS: 7683-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-207.40	kJ/mol	Joback Method
hf	-497.78	kJ/mol	Joback Method
hfus	31.99	kJ/mol	Joback Method
hvap	90.72	kJ/mol	Joback Method
log10ws	0.14		Aqueous Solubility Prediction Method
logp	1.129		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	780.47	K	Joback Method
tc	996.60	K	Joback Method

tf	437.98	K	Aqueous Solubility Prediction Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.82	J/mol×K	780.47	Joback Method
cpg	517.72	J/mol×K	816.49	Joback Method
cpg	528.22	J/mol×K	852.51	Joback Method
cpg	538.47	J/mol×K	888.53	Joback Method
cpg	548.57	J/mol×K	924.56	Joback Method
cpg	558.64	J/mol×K	960.58	Joback Method
cpg	568.81	J/mol×K	996.60	Joback Method

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=C7683592&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
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