ISOXUPRINE

Other names: Benzenemethanol, 4-hydroxy-«alpha»-[1-[(1-methyl-2-phenoxyethyl)amino]ethyl]-
Benzyl alcohol, p-hydroxy-«alpha»-(1-((1-methyl-2-phenoxyethyl)amino)ethyl)-
Dilavase
p-Hydroxy-N-(1-methyl-2-phenoxyethyl)norephedrine
1-(4-Hydroxyphenyl)-2-(1-methyl-2-phenoxyethylamino)propanol
Vasodilian
Isoxuprine
4-Hydroxy-«alpha»-[1-[(1-methyl-2-phenoxyethyl)amino]ethyl]benzyl alcohol
1-(p-Hydroxyphenyl)-2-(1-methyl-2-phenoxyethylamino)-1-propanol
2-(3-Phenoxy-2-propylamino)-1-(p-hydroxyphenyl)-1-propanol
erythro-1-(p-Hydroxyphenyl)-2-(«alpha»-methyl-«beta»-phenoxyethylamino)propanol
p-Hydroxy-«alpha»-(1-((1-methyl-2-phenoxyethyl)amino)ethyl)benzyl alcohol
isoxysuprine

Inchi: InChI=1S/C18H23NO3/c1-13(12-22-17-6-4-3-5-7-17)19-14(2)18(21)15-8-10-16(20)11-9-

InchiKey: BMUKKTUHUDJSNZ-UHFFFAOYSA-N

Formula: C18H23NO3

SMILES: CC(COc1ccccc1)NC(C)C(O)c1ccc(O)cc1

Mol. weight [g/mol]: 301.39

Physical Properties

Property code	Value	Unit	Source
hfus	36.05	kJ/mol	Joback Method
logp	2.871		Crippen Method
mcvol	244.550	ml/mol	McGowan Method
rinpol	2314.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	662.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	777.39	J/mol×K	908.67	Joback Method
cpg	790.91	J/mol×K	946.26	Joback Method
cpg	803.71	J/mol×K	983.85	Joback Method
cpg	815.89	J/mol×K	1021.43	Joback Method
cpg	827.58	J/mol×K	1059.02	Joback Method
cpg	838.89	J/mol×K	1096.61	Joback Method
cpg	849.92	J/mol×K	1134.20	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C395288&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature