2-Propanol, 1-(1H-indol-4-yloxy)-3-[(1-methylethyl)amino]-

Other names: (.+/-.)-Pindolol
(±) 1-(1H-indol-4-yloxy)-3-(isopropylamino)-2-propanol (pindolol)
1-(1H-Indol-4-yloxy)-3-((1-methylethyl)amino)-2-propanol
1-(1H-indol-4-yloxy)-3-(propan-2-ylamino)propan-2-ol
1-(4-Indolyloxy)-3-(isopropylamino)-2-propanol
1-(Indol-4-yloxy)-3-(isopropylamino)-2-propanol
2-Propanol, 1-(4-indolyloxy)-3-(isopropylamino)-
4-(2-Hydroxy-3-isopropylaminopropoxy)-indole
4-(3-(Isopropylamino)-2-hydroxypropoxy)indole
Betapindol
Blockin L
Blocklin L
Calvisken
Carvisken
Decreten
Durapindol
Glauco-Visken
LB-46
Pectobloc
Pinbetol
Prinodolol
Pynastin
Visken
pindolol

Inchi: InChI=1S/C14H20N2O2/c1-10(2)16-8-11(17)9-18-14-5-3-4-13-12(14)6-7-15-13/h3-7,10-1

InchiKey: JZQKKSLKJUAGIC-UHFFFAOYSA-N

Formula: C14H20N2O2

SMILES: CC(C)NCC(O)COc1cccc2[nH]ccc12

Mol. weight [g/mol]: 248.33

Physical Properties

Property code	Value	Unit	Source
hsub	146.00 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.58		Aqueous Solubility Prediction Method
logp	1.424		Crippen Method
mcvol	200.900	ml/mol	McGowan Method

rinpol	2273.00		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2231.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2261.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tf	290.00 ± 0.60	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	60.60	kJ/mol	423.60	NIST Webbook
hfust	58.00	kJ/mol	443.80	NIST Webbook
hfust	57.90	kJ/mol	442.90	NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Solubility and Salting Behavior of Several ?-Adrenergic Blocking Agents in Liquid and Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je0497202

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13523869&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point