Oxprenolol

Other names: 1-((1-Methylethyl)amino)-3-(2-(2-propenyloxy)phenoxy)-2-propanol
1-(Isopropylamino)-2-hydroxy-3-(o-(allyloxy)phenoxy)propane
1-(o-(Allyloxy)phenoxy)-3-(isopropylamino)-2-propanol
2-Propanol, 1-(2-allyloxyphenoxy)-3-(isopropylamino)-
2-Propanol, 1-[(1-methylethyl)amino]-3-[2-(2-propenyloxy)phenoxy]-
Coretal

Inchi: InChI=1S/C15H23NO3/c1-4-9-18-14-7-5-6-8-15(14)19-11-13(17)10-16-12(2)3/h4-8,12-13

InchiKey: CEMAWMOMDPGJMB-UHFFFAOYSA-N

Formula: C15H23NO3

SMILES: C=CCOc1ccccc1OCC(O)CNC(C)C

Mol. weight [g/mol]: 265.35

CAS: 6452-71-7

Physical Properties

Property code	Value	Unit	Source
gf	3.73	kJ/mol	Joback Method
hf	-376.20	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	78.41	kJ/mol	Joback Method
log10ws	0.38		Aqueous Solubility Prediction Method
logp	1.989		Crippen Method
mcvol	221.740	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	757.25	K	Joback Method
tc	950.55	K	Joback Method
tf	385.00	K	Aqueous Solubility Prediction Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.81	J/mol×K	757.25	Joback Method
cpg	664.07	J/mol×K	789.47	Joback Method
cpg	677.46	J/mol×K	821.68	Joback Method
cpg	690.00	J/mol×K	853.90	Joback Method
cpg	701.71	J/mol×K	886.12	Joback Method
cpg	712.62	J/mol×K	918.34	Joback Method
cpg	722.73	J/mol×K	950.55	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6452717&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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