Bisoprolol

Other names:	2-Propanol, 1-[4-[[2-(1-methylethoxy)ethoxy]methyl]phenoxy]-3-[(1-methylethyl)amino]-, (.+/-.)- (.+/-.)-1-[[«alpha»-(2-isopropoxyethoxy)-p-tolyl]oxy]-3-(isopropylamino)-2-propanol EMD-33512 Bisoprolol - from tablet donated by Watson - Bisprolol 2-Propanol, 1-[4-[[2-(1-methylethoxy)ethoxy]methyl]phenoxy]-3-[(1-methylethyl)amino]- 1-(p-2-isopropoxyethoxymethylphenoxy)-3-isopropylaminopropan-2-ol
Inchi:	InChI=1S/C18H31NO4/c1-14(2)19-11-17(20)13-23-18-7-5-16(6-8-18)12-21-9-10-22-15(3
InchiKey:	VHYCDWMUTMEGQY-UHFFFAOYSA-N
Formula:	C18H31NO4
SMILES:	CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1
Mol. weight [g/mol]:	325.44
CAS:	66722-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-166.29	kJ/mol	Joback Method
hf	-701.05	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.366		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
tb	851.19	K	Joback Method
tc	1047.85	K	Joback Method
tf	466.73	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.57	J/mol×K	851.19	Joback Method
cpg	893.08	J/mol×K	883.97	Joback Method

cpg	907.47	J/mol×K	916.74	Joback Method
cpg	920.76	J/mol×K	949.52	Joback Method
cpg	932.94	J/mol×K	982.30	Joback Method
cpg	944.05	J/mol×K	1015.08	Joback Method
cpg	954.08	J/mol×K	1047.85	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66722449&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume