Propranolol hydroxy, acetylated

Inchi: InChI=1S/C22H27NO6/c1-14(2)23(15(3)24)12-18(28-16(4)25)13-27-21-10-11-22(29-17(5
InchiKey: BTJVNFSGLYHZFD-UHFFFAOYSA-N
Formula: C22H27NO6
SMILES: CC(=O)Oc1ccc(OCC(CN(C(C)=O)C(C)C)OC(C)=O)c2ccccc12
Mol. weight [g/mol]: 401.45

Physical Properties

Property code	Value	Unit	Source
gf	-261.70	kJ/mol	Joback Method
hf	-770.18	kJ/mol	Joback Method
hfus	47.35	kJ/mol	Joback Method
hvap	98.54	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.332		Crippen Method
mcvol	309.920	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2940.00		NIST Webbook
tb	998.81	K	Joback Method
tc	1227.16	K	Joback Method
tf	640.81	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.20	J/mol×K	998.81	Joback Method
cpg	1012.41	J/mol×K	1036.87	Joback Method
cpg	1023.28	J/mol×K	1074.93	Joback Method
cpg	1032.86	J/mol×K	1112.98	Joback Method
cpg	1041.19	J/mol×K	1151.04	Joback Method
cpg	1048.34	J/mol×K	1189.10	Joback Method
cpg	1054.35	J/mol×K	1227.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583001&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