2-Acetoxy-1-(N-acetyl-N-isopropyl)amino-3-[4-(2-c

Other names: Betaxolol, acetylated
Inchi: InChI=1S/C22H33NO5/c1-16(2)23(17(3)24)13-22(28-18(4)25)15-27-21-9-7-19(8-10-21)1
InchiKey: LCDAJZUFFYUMTM-UHFFFAOYSA-N
Formula: C22H33NO5
SMILES: CC(=O)OC(COc1ccc(CCOCC2CC2)cc1)CN(C(C)=O)C(C)C
Mol. weight [g/mol]: 391.50
CAS: 169613-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-169.05	kJ/mol	Joback Method
hf	-764.40	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	89.41	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.223		Crippen Method
mcvol	316.950	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	927.72	K	Joback Method
tc	1141.14	K	Joback Method
tf	563.60	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.74	J/mol×K	927.72	Joback Method
cpg	1069.87	J/mol×K	963.29	Joback Method
cpg	1084.69	J/mol×K	998.86	Joback Method
cpg	1098.27	J/mol×K	1034.43	Joback Method
cpg	1110.65	J/mol×K	1070.00	Joback Method
cpg	1121.89	J/mol×K	1105.57	Joback Method

cpg	1132.05	J/mol×K	1141.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C169613961&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume