1-(2-Acetoxyethyl)-4-[2-acetoxy-3-acetyl(isopropy

Other names: Betaxolol, O-desalkyl, acetylated
Inchi: InChI=1S/C20H29NO6/c1-14(2)21(15(3)22)12-20(27-17(5)24)13-26-19-8-6-18(7-9-19)10
InchiKey: FNJVJYPQOZGHTN-UHFFFAOYSA-N
Formula: C20H29NO6
SMILES: CC(=O)OCCc1ccc(OCC(CN(C(C)=O)C(C)C)OC(C)=O)cc1
Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-375.56	kJ/mol	Joback Method
hf	-908.50	kJ/mol	Joback Method
hfus	45.54	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.360		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
tb	929.09	K	Joback Method
tc	1142.66	K	Joback Method
tf	573.05	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.24	J/mol×K	929.09	Joback Method
cpg	978.98	J/mol×K	964.68	Joback Method
cpg	991.34	J/mol×K	1000.28	Joback Method
cpg	1002.31	J/mol×K	1035.87	Joback Method
cpg	1011.94	J/mol×K	1071.47	Joback Method
cpg	1020.23	J/mol×K	1107.06	Joback Method
cpg	1027.22	J/mol×K	1142.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U280809&Units=SI

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