1-(2-Acetoxyethyl)-4-[3-acetyl(isopropyl)aminopro

Other names: Betaxolol, O-desalkyl - H2O, acetylated
Inchi: InChI=1S/C18H25NO4/c1-14(2)19(15(3)20)11-5-12-23-18-8-6-17(7-9-18)10-13-22-16(4)
InchiKey: VNGUHMDNAOOLBY-VZUCSPMQSA-N
Formula: C18H25NO4
SMILES: CC(=O)OCCc1ccc(OCC=CN(C(C)=O)C(C)C)cc1
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
gf	-75.82	kJ/mol	Joback Method
hf	-499.92	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.942		Crippen Method
mcvol	261.280	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2570.00		NIST Webbook
tb	811.64	K	Joback Method
tc	1017.86	K	Joback Method
tf	488.27	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.64	J/mol×K	811.64	Joback Method
cpg	793.03	J/mol×K	846.01	Joback Method
cpg	807.36	J/mol×K	880.38	Joback Method
cpg	820.65	J/mol×K	914.75	Joback Method
cpg	832.95	J/mol×K	949.12	Joback Method
cpg	844.30	J/mol×K	983.49	Joback Method
cpg	854.73	J/mol×K	1017.86	Joback Method

Sources

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=U280810&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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