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

Other names: Alprenolol, hydroxy, acetylated
Inchi: InChI=1S/C21H29NO6/c1-7-8-18-11-19(27-16(5)24)9-10-21(18)26-13-20(28-17(6)25)12-
InchiKey: LBOSTHQFSRFOGE-UHFFFAOYSA-N
Formula: C21H29NO6
SMILES: C=CCc1cc(OC(C)=O)ccc1OCC(CN(C(C)=O)C(C)C)OC(C)=O
Mol. weight [g/mol]: 391.46

Physical Properties

Property code	Value	Unit	Source
gf	-288.93	kJ/mol	Joback Method
hf	-815.18	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	2.908		Crippen Method
mcvol	310.990	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2575.00		NIST Webbook
tb	953.63	K	Joback Method
tc	1171.02	K	Joback Method
tf	595.08	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.53	J/mol×K	953.63	Joback Method
cpg	1007.82	J/mol×K	989.86	Joback Method
cpg	1019.69	J/mol×K	1026.09	Joback Method
cpg	1030.16	J/mol×K	1062.33	Joback Method
cpg	1039.25	J/mol×K	1098.56	Joback Method
cpg	1046.99	J/mol×K	1134.79	Joback Method
cpg	1053.40	J/mol×K	1171.02	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=U281340&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

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