Acebutolol hydrolysed, acetylated

Inchi: InChI=1S/C20H28N2O6/c1-12(2)22(15(5)25)10-18(28-16(6)26)11-27-20-8-7-17(21-14(4)
InchiKey: UQJURMOWYXOGDP-UHFFFAOYSA-N
Formula: C20H28N2O6
SMILES: CC(=O)Nc1ccc(OCC(CN(C(C)=O)C(C)C)OC(C)=O)c(C(C)=O)c1
Mol. weight [g/mol]: 392.45

Physical Properties

Property code	Value	Unit	Source
gf	-319.72	kJ/mol	Joback Method
hf	-846.86	kJ/mol	Joback Method
hfus	50.66	kJ/mol	Joback Method
hvap	103.22	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.415		Crippen Method
mcvol	306.880	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	1015.69	K	Joback Method
tc	1244.67	K	Joback Method
tf	665.93	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.60	J/mol×K	1015.69	Joback Method
cpg	1011.68	J/mol×K	1053.85	Joback Method
cpg	1021.30	J/mol×K	1092.02	Joback Method
cpg	1029.47	J/mol×K	1130.18	Joback Method
cpg	1036.25	J/mol×K	1168.34	Joback Method
cpg	1041.66	J/mol×K	1206.50	Joback Method
cpg	1045.74	J/mol×K	1244.67	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=R582395&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