Carteolol hydroxy, acetylated

Inchi: InChI=1S/C23H32N2O7/c1-14(26)25(23(4,5)6)12-11-17(31-15(2)27)13-30-19-8-9-20(32-
InchiKey: RUQKNCGDKVIFJX-UHFFFAOYSA-N
Formula: C23H32N2O7
SMILES: CC(=O)Oc1ccc(OCC(CCN(C(C)=O)C(C)(C)C)OC(C)=O)c2c1NC(=O)CC2
Mol. weight [g/mol]: 448.51

Physical Properties

Property code	Value	Unit	Source
gf	-342.80	kJ/mol	Joback Method
hf	-1009.74	kJ/mol	Joback Method
hfus	52.71	kJ/mol	Joback Method
hvap	110.28	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	2.844		Crippen Method
mcvol	344.160	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	1136.95	K	Joback Method
tc	1391.95	K	Joback Method
tf	841.23	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.17	J/mol×K	1136.95	Joback Method
cpg	1195.28	J/mol×K	1179.45	Joback Method
cpg	1201.27	J/mol×K	1221.95	Joback Method
cpg	1205.17	J/mol×K	1264.45	Joback Method
cpg	1207.01	J/mol×K	1306.95	Joback Method
cpg	1206.84	J/mol×K	1349.45	Joback Method
cpg	1204.69	J/mol×K	1391.95	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=R582602&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

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