Carteolol, acetylated

Inchi: InChI=1S/C21H30N2O5/c1-14(24)23(21(3,4)5)12-11-16(28-15(2)25)13-27-19-8-6-7-18-1
InchiKey: TYXHTZYLZMBLJV-UHFFFAOYSA-N
Formula: C21H30N2O5
SMILES: CC(=O)OC(CCN(C(C)=O)C(C)(C)C)COc1cccc2c1CCC(=O)N2
Mol. weight [g/mol]: 390.47

Physical Properties

Property code	Value	Unit	Source
gf	-116.09	kJ/mol	Joback Method
hf	-712.19	kJ/mol	Joback Method
hfus	45.13	kJ/mol	Joback Method
hvap	96.01	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.919		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	1009.92	K	Joback Method
tc	1245.42	K	Joback Method
tf	734.01	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.98	J/mol×K	1009.92	Joback Method
cpg	1055.10	J/mol×K	1049.17	Joback Method
cpg	1066.66	J/mol×K	1088.42	Joback Method
cpg	1076.72	J/mol×K	1127.67	Joback Method
cpg	1085.33	J/mol×K	1166.92	Joback Method
cpg	1092.54	J/mol×K	1206.17	Joback Method
cpg	1098.41	J/mol×K	1245.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582593&Units=SI
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

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