Oxprenolol hydroxy , isomer I, acetylated

Inchi: InChI=1S/C22H31NO6/c1-7-12-27-22-13-20(28-17(5)25)10-8-19(22)9-11-21(29-18(6)26)
InchiKey: VTVKNVJHWVSJMJ-UHFFFAOYSA-N
Formula: C22H31NO6
SMILES: C=CCOc1cc(OC(C)=O)ccc1CCC(CN(C(C)=O)C(C)C)OC(C)=O
Mol. weight [g/mol]: 405.48

Physical Properties

Property code	Value	Unit	Source
gf	-280.51	kJ/mol	Joback Method
hf	-835.82	kJ/mol	Joback Method
hfus	49.05	kJ/mol	Joback Method
hvap	96.23	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.298		Crippen Method
mcvol	325.080	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	976.51	K	Joback Method
tc	1196.89	K	Joback Method
tf	606.35	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.16	J/mol×K	976.51	Joback Method
cpg	1067.52	J/mol×K	1013.24	Joback Method
cpg	1079.38	J/mol×K	1049.97	Joback Method
cpg	1089.78	J/mol×K	1086.70	Joback Method
cpg	1098.74	J/mol×K	1123.43	Joback Method
cpg	1106.28	J/mol×K	1160.16	Joback Method
cpg	1112.44	J/mol×K	1196.89	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582860&Units=SI

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