Toliprolol hydroxy, acetylated

Inchi: InChI=1S/C19H27NO6/c1-12(2)20(14(4)21)10-18(25-15(5)22)11-24-17-7-8-19(13(3)9-17
InchiKey: REVONIZMEPYZLV-UHFFFAOYSA-N
Formula: C19H27NO6
SMILES: CC(=O)Oc1ccc(OCC(CN(C(C)=O)C(C)C)OC(C)=O)cc1C
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-393.61	kJ/mol	Joback Method
hf	-899.33	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	90.22	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.488		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	911.19	K	Joback Method
tc	1124.03	K	Joback Method
tf	574.30	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.24	J/mol×K	911.19	Joback Method
cpg	918.78	J/mol×K	946.66	Joback Method
cpg	930.98	J/mol×K	982.14	Joback Method
cpg	941.84	J/mol×K	1017.61	Joback Method
cpg	951.36	J/mol×K	1053.08	Joback Method
cpg	959.57	J/mol×K	1088.56	Joback Method
cpg	966.46	J/mol×K	1124.03	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=R583105&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