Toliprolol desamino dihydroxy, acetylated

Inchi: InChI=1S/C16H20O7/c1-10-7-14(5-6-16(10)23-13(4)19)21-9-15(22-12(3)18)8-20-11(2)17
InchiKey: STFZMNIVKHKFDP-UHFFFAOYSA-N
Formula: C16H20O7
SMILES: CC(=O)OCC(COc1ccc(OC(C)=O)c(C)c1)OC(C)=O
Mol. weight [g/mol]: 324.33

Physical Properties

Property code	Value	Unit	Source
gf	-632.21	kJ/mol	Joback Method
hf	-1031.88	kJ/mol	Joback Method
hfus	36.48	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.794		Crippen Method
mcvol	240.730	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2200.00		NIST Webbook
tb	852.97	K	Joback Method
tc	1064.05	K	Joback Method
tf	545.25	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.59	J/mol×K	852.97	Joback Method
cpg	730.12	J/mol×K	888.15	Joback Method
cpg	741.44	J/mol×K	923.33	Joback Method
cpg	751.52	J/mol×K	958.51	Joback Method
cpg	760.33	J/mol×K	993.69	Joback Method
cpg	767.85	J/mol×K	1028.87	Joback Method
cpg	774.06	J/mol×K	1064.05	Joback Method
dvisc	0.0003541	Pa×s	545.25	Joback Method
dvisc	0.0002202	Pa×s	596.54	Joback Method

dvisc	0.0001476	Pa×s	647.82	Joback Method
dvisc	0.0001050	Pa×s	699.11	Joback Method
dvisc	0.0000782	Pa×s	750.40	Joback Method
dvisc	0.0000605	Pa×s	801.68	Joback Method
dvisc	0.0000482	Pa×s	852.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583076&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
dvisc:	Dynamic viscosity
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