Oxprenolol desamino, hydroxy, desalkyl - H2O, acetylated

Inchi: InChI=1S/C14H16O4/c1-11(15)17-10-6-5-8-13-7-3-4-9-14(13)18-12(2)16/h3-7,9H,8,10H2

InchiKey: CGXXIBNEDSBELJ-AATRIKPKSA-N

Formula: C14H16O4

SMILES: CC(=O)OCC=CCc1ccccc1OC(C)=O

Mol. weight [g/mol]: 248.27

Physical Properties

Property code	Value	Unit	Source
gf	-217.84	kJ/mol	Joback Method
hf	-479.61	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.274		Crippen Method
mcvol	194.940	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1920.00		NIST Webbook
tb	708.12	K	Joback Method
tc	921.39	K	Joback Method
tf	425.72	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.56	J/mol×K	708.12	Joback Method
cpg	576.79	J/mol×K	885.84	Joback Method
cpg	566.47	J/mol×K	850.30	Joback Method
cpg	555.31	J/mol×K	814.75	Joback Method
cpg	543.28	J/mol×K	779.21	Joback Method
cpg	530.37	J/mol×K	743.66	Joback Method
cpg	586.30	J/mol×K	921.39	Joback Method
dvisc	0.0001029	Pa×s	708.12	Joback Method
dvisc	0.0001299	Pa×s	661.05	Joback Method

dvisc	0.0001701	Pa×s	613.99	Joback Method
dvisc	0.0002329	Pa×s	566.92	Joback Method
dvisc	0.0003376	Pa×s	519.85	Joback Method
dvisc	0.0005268	Pa×s	472.79	Joback Method
dvisc	0.0009071	Pa×s	425.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582835&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