Alprenolol desaminohydroxy, acetylated

Inchi: InChI=1S/C16H20O5/c1-4-7-14-8-5-6-9-16(14)20-11-15(21-13(3)18)10-19-12(2)17/h4-6,
InchiKey: HPBBAFJJVJUGNE-UHFFFAOYSA-N
Formula: C16H20O5
SMILES: C=CCc1ccccc1OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-300.82	kJ/mol	Joback Method
hf	-650.18	kJ/mol	Joback Method
hfus	32.81	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.289		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1850.00		NIST Webbook
tb	768.38	K	Joback Method
tc	974.88	K	Joback Method
tf	458.81	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.33	J/mol×K	768.38	Joback Method
cpg	665.76	J/mol×K	802.80	Joback Method
cpg	679.16	J/mol×K	837.21	Joback Method
cpg	691.54	J/mol×K	871.63	Joback Method
cpg	702.91	J/mol×K	906.05	Joback Method
cpg	713.26	J/mol×K	940.46	Joback Method
cpg	722.60	J/mol×K	974.88	Joback Method
dvisc	0.0007018	Pa×s	458.81	Joback Method
dvisc	0.0003931	Pa×s	510.41	Joback Method

dvisc	0.0002449	Pa×s	562.00	Joback Method
dvisc	0.0001652	Pa×s	613.60	Joback Method
dvisc	0.0001185	Pa×s	665.19	Joback Method
dvisc	0.0000891	Pa×s	716.79	Joback Method
dvisc	0.0000697	Pa×s	768.38	Joback Method

Sources

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=R582444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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