Alprenolol desaminodihydroxy, acetylated

Inchi: InChI=1S/C18H22O7/c1-5-6-15-9-16(24-13(3)20)7-8-18(15)23-11-17(25-14(4)21)10-22-1
InchiKey: UGLDVYYRPLVKDT-UHFFFAOYSA-N
Formula: C18H22O7
SMILES: C=CCc1cc(OC(C)=O)ccc1OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 350.36

Physical Properties

Property code	Value	Unit	Source
gf	-527.53	kJ/mol	Joback Method
hf	-947.73	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	88.08	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.214		Crippen Method
mcvol	264.610	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	895.41	K	Joback Method
tc	1108.27	K	Joback Method
tf	566.03	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/mol×K	895.41	Joback Method
cpg	816.24	J/mol×K	930.89	Joback Method
cpg	827.24	J/mol×K	966.36	Joback Method
cpg	836.91	J/mol×K	1001.84	Joback Method
cpg	845.25	J/mol×K	1037.32	Joback Method
cpg	852.24	J/mol×K	1072.80	Joback Method
cpg	857.86	J/mol×K	1108.27	Joback Method
dvisc	0.0002990	Pa×s	566.03	Joback Method

dvisc	0.0001832	Pa×s	620.93	Joback Method
dvisc	0.0001216	Pa×s	675.82	Joback Method
dvisc	0.0000858	Pa×s	730.72	Joback Method
dvisc	0.0000636	Pa×s	785.62	Joback Method
dvisc	0.0000490	Pa×s	840.51	Joback Method
dvisc	0.0000390	Pa×s	895.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582424&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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