2-deoxyribitol, acetylated

Inchi: InChI=1S/C13H20O8/c1-8(14)18-6-5-12(20-10(3)16)13(21-11(4)17)7-19-9(2)15/h12-13H
InchiKey: PSLLPAIVUVLGNH-UHFFFAOYSA-N
Formula: C13H20O8
SMILES: CC(=O)OCCC(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 304.29

Physical Properties

Property code	Value	Unit	Source
gf	-881.98	kJ/mol	Joback Method
hf	-1301.41	kJ/mol	Joback Method
hfus	33.53	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.366		Crippen Method
mcvol	223.790	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1681.80		NIST Webbook
tb	801.12	K	Joback Method
tc	997.63	K	Joback Method
tf	494.91	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.07	J/mol×K	801.12	Joback Method
cpg	673.51	J/mol×K	833.87	Joback Method
cpg	684.98	J/mol×K	866.62	Joback Method
cpg	695.46	J/mol×K	899.37	Joback Method
cpg	704.92	J/mol×K	932.13	Joback Method
cpg	713.33	J/mol×K	964.88	Joback Method
cpg	720.67	J/mol×K	997.63	Joback Method
dvisc	0.0006776	Pa×s	494.91	Joback Method
dvisc	0.0003785	Pa×s	545.94	Joback Method

dvisc	0.0002335	Pa×s	596.98	Joback Method
dvisc	0.0001555	Pa×s	648.01	Joback Method
dvisc	0.0001099	Pa×s	699.05	Joback Method
dvisc	0.0000814	Pa×s	750.09	Joback Method
dvisc	0.0000626	Pa×s	801.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R488847&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