Glucose, 2,3,6-trimethyl, acetylated

Inchi: InChI=1S/C13H22O8/c1-7(14)19-10-9(6-16-3)21-13(20-8(2)15)12(18-5)11(10)17-4/h9-13
InchiKey: HXLRYGRACUTNDH-WJTVCTBASA-N
Formula: C13H22O8
SMILES: COCC1OC(OC(C)=O)C(OC)C(OC)C1OC(C)=O
Mol. weight [g/mol]: 306.31

Physical Properties

Property code	Value	Unit	Source
gf	-816.77	kJ/mol	Joback Method
hf	-1356.95	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	-0.118		Crippen Method
mcvol	221.530	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1995.00		NIST Webbook
tb	744.50	K	Joback Method
tc	941.85	K	Joback Method
tf	464.27	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.63	J/mol×K	744.50	Joback Method
cpg	708.87	J/mol×K	777.39	Joback Method
cpg	724.93	J/mol×K	810.28	Joback Method
cpg	739.76	J/mol×K	843.18	Joback Method
cpg	753.30	J/mol×K	876.07	Joback Method
cpg	765.49	J/mol×K	908.96	Joback Method
cpg	776.29	J/mol×K	941.85	Joback Method
dvisc	0.0006779	Pa×s	464.27	Joback Method
dvisc	0.0004575	Pa×s	510.97	Joback Method

dvisc	0.0003297	Pa×s	557.68	Joback Method
dvisc	0.0002500	Pa×s	604.38	Joback Method
dvisc	0.0001972	Pa×s	651.09	Joback Method
dvisc	0.0001606	Pa×s	697.80	Joback Method
dvisc	0.0001342	Pa×s	744.50	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=R530082&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