Glucose, 3,6-dimethyl, nitrile, acetylated

Inchi: InChI=1S/C14H21NO8/c1-8(16)21-11(6-15)13(20-5)14(23-10(3)18)12(7-19-4)22-9(2)17/
InchiKey: CODTYEMFRJDDAD-REWJHTLYSA-N
Formula: C14H21NO8
SMILES: COCC(OC(C)=O)C(OC(C)=O)C(OC)C(C#N)OC(C)=O
Mol. weight [g/mol]: 331.32

Physical Properties

Property code	Value	Unit	Source
gf	-721.34	kJ/mol	Joback Method
hf	-1187.37	kJ/mol	Joback Method
hfus	30.17	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	-0.034		Crippen Method
mcvol	243.560	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	893.75	K	Joback Method
tc	1102.82	K	Joback Method
tf	513.47	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.88	J/mol×K	893.75	Joback Method
cpg	761.71	J/mol×K	928.60	Joback Method
cpg	771.24	J/mol×K	963.44	Joback Method
cpg	779.42	J/mol×K	998.29	Joback Method
cpg	786.22	J/mol×K	1033.13	Joback Method
cpg	791.60	J/mol×K	1067.98	Joback Method
cpg	795.52	J/mol×K	1102.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530255&Units=SI

Legend

cpg:	Ideal gas heat capacity
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