Glucose, 2,3,6-triethyl, nitrile, acetylated

Inchi: InChI=1S/C16H27NO7/c1-6-20-10-14(23-11(4)18)16(24-12(5)19)15(22-8-3)13(9-17)21-7
InchiKey: VFGSUILNLCLZPY-ZJIFWQFVSA-N
Formula: C16H27NO7
SMILES: CCOCC(OC(C)=O)C(OC(C)=O)C(OCC)C(C#N)OCC
Mol. weight [g/mol]: 345.39

Physical Properties

Property code	Value	Unit	Source
gf	-575.58	kJ/mol	Joback Method
hf	-1116.07	kJ/mol	Joback Method
hfus	33.75	kJ/mol	Joback Method
hvap	85.68	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.220		Crippen Method
mcvol	270.170	ml/mol	McGowan Method
pc	1365.67	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	885.64	K	Joback Method
tc	1089.27	K	Joback Method
tf	486.08	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.87	J/mol×K	885.64	Joback Method
cpg	868.04	J/mol×K	919.58	Joback Method
cpg	879.90	J/mol×K	953.52	Joback Method
cpg	890.41	J/mol×K	987.45	Joback Method
cpg	899.56	J/mol×K	1021.39	Joback Method
cpg	907.30	J/mol×K	1055.33	Joback Method
cpg	913.62	J/mol×K	1089.27	Joback Method

Sources

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=R530077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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