Glucose, 3-ethyl, nitrile, acetylated

Inchi: InChI=1S/C16H23NO9/c1-6-22-15(13(7-17)24-10(3)19)16(26-12(5)21)14(25-11(4)20)8-2
InchiKey: ZSXLAXDLHWREBI-ZJIFWQFVSA-N
Formula: C16H23NO9
SMILES: CCOC(C(C#N)OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 373.36

Physical Properties

Property code	Value	Unit	Source
gf	-833.42	kJ/mol	Joback Method
hf	-1341.23	kJ/mol	Joback Method
hfus	36.95	kJ/mol	Joback Method
hvap	99.17	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	0.273		Crippen Method
mcvol	273.310	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	993.38	K	Joback Method
tc	1216.96	K	Joback Method
tf	585.94	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.38	J/mol×K	993.38	Joback Method
cpg	878.74	J/mol×K	1030.64	Joback Method
cpg	885.36	J/mol×K	1067.91	Joback Method
cpg	890.18	J/mol×K	1105.17	Joback Method
cpg	893.17	J/mol×K	1142.44	Joback Method
cpg	894.29	J/mol×K	1179.70	Joback Method

cpg	893.48	J/mol×K	1216.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530275&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

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