Glucose, 3,6-diethyl, nitrile, acetylated

Inchi: InChI=1S/C16H25NO8/c1-6-21-9-14(24-11(4)19)16(25-12(5)20)15(22-7-2)13(8-17)23-10
InchiKey: RLKCMBWIPKIYPQ-ZJIFWQFVSA-N
Formula: C16H25NO8
SMILES: CCOCC(OC(C)=O)C(OC(C)=O)C(OCC)C(C#N)OC(C)=O
Mol. weight [g/mol]: 359.37

Physical Properties

Property code	Value	Unit	Source
gf	-704.50	kJ/mol	Joback Method
hf	-1228.65	kJ/mol	Joback Method
hfus	35.35	kJ/mol	Joback Method
hvap	92.42	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	0.747		Crippen Method
mcvol	271.740	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	939.51	K	Joback Method
tc	1152.73	K	Joback Method
tf	536.01	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.23	J/mol×K	939.51	Joback Method
cpg	876.18	J/mol×K	975.05	Joback Method
cpg	885.62	J/mol×K	1010.58	Joback Method
cpg	893.52	J/mol×K	1046.12	Joback Method
cpg	899.84	J/mol×K	1081.65	Joback Method
cpg	904.54	J/mol×K	1117.19	Joback Method

cpg	907.58	J/mol×K	1152.73	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=R530235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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