

# Glucose, 2-ethyl, nitrile, acetylated

<b>Inchi:</b>	InChI=1S/C16H23NO9/c1-6-22-13(7-17)15(25-11(4)20)16(26-12(5)21)14(24-10(3)19)8-2
<b>InchiKey:</b>	VYXVHDPIABFEFM-ZJIFWQFVSA-N
<b>Formula:</b>	C16H23NO9
<b>SMILES:</b>	CCOC(C#N)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
<b>Mol. weight [g/mol]:</b>	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	2054.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2050.00		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/molxK	993.38	Joback Method
cpg	878.74	J/molxK	1030.64	Joback Method
cpg	885.36	J/molxK	1067.91	Joback Method
cpg	890.18	J/molxK	1105.17	Joback Method
cpg	893.17	J/molxK	1142.44	Joback Method
cpg	894.29	J/molxK	1179.70	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R530191&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R530191&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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