

# Glucose, nitrile, acetylated

<b>Inchi:</b>	InChI=1S/C16H21NO10/c1-8(18)23-7-14(25-10(3)20)16(27-12(5)22)15(26-11(4)21)13(6
<b>InchiKey:</b>	INCBLRCTSZYSJE-ZJIFWQFVSA-N
<b>Formula:</b>	C16H21NO10
<b>SMILES:</b>	CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(C#N)OC(C)=O
<b>Mol. weight [g/mol]:</b>	387.34

## Physical Properties

Property code	Value	Unit	Source
gf	-962.34	kJ/mol	Joback Method
hf	-1453.81	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	105.92	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	-0.200		Crippen Method
mcvol	274.880	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	1047.25	K	Joback Method
tc	1282.15	K	Joback Method
tf	635.87	K	Joback Method
vc	1.054	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.07	J/molxK	1047.25	Joback Method
cpg	875.40	J/molxK	1086.40	Joback Method
cpg	878.69	J/molxK	1125.55	Joback Method
cpg	879.90	J/molxK	1164.70	Joback Method

cpg	878.96	J/mol×K	1203.85	Joback Method
cpg	875.84	J/mol×K	1243.00	Joback Method
cpg	870.46	J/mol×K	1282.15	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R530057&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R530057&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

## 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>hvp:</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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