

# Glucose, 3-methyl, nitrile, acetylated

**Inchi:** InChI=1S/C15H21NO9/c1-8(17)22-7-13(24-10(3)19)15(25-11(4)20)14(21-5)12(6-16)23-9  
**InchiKey:** RWCWXRUZHPANFS-GBJTYRQASA-N  
**Formula:** C15H21NO9  
**SMILES:** COC(C(C#N)OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O  
**Mol. weight [g/mol]:** 359.33

## Physical Properties

Property code	Value	Unit	Source
gf	-841.84	kJ/mol	Joback Method
hf	-1320.59	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	96.94	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	-0.117		Crippen Method
mcvol	259.220	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2071.00		NIST Webbook
rinpol	2069.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	970.50	K	Joback Method
tc	1190.72	K	Joback Method
tf	574.67	K	Joback Method
vc	0.992	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.47	J/molxK	970.50	Joback Method
cpg	821.94	J/molxK	1007.20	Joback Method
cpg	828.78	J/molxK	1043.91	Joback Method
cpg	833.96	J/molxK	1080.61	Joback Method
cpg	837.44	J/molxK	1117.32	Joback Method
cpg	839.16	J/molxK	1154.02	Joback Method
cpg	839.08	J/molxK	1190.72	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R530295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R530295&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>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>rinp:</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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