

# 2-deoxyglucitol, acetylated

<b>Inchi:</b>	InChI=1S/C16H24O10/c1-9(17)22-7-6-14(24-11(3)19)16(26-13(5)21)15(25-12(4)20)8-23
<b>InchiKey:</b>	WXCAGOPORGCRJM-UHFFFAOYSA-N
<b>Formula:</b>	C16H24O10
<b>SMILES:</b>	CC(=O)OCCC(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
<b>Mol. weight [g/mol]:</b>	376.36

## Physical Properties

Property code	Value	Unit	Source
gf	-1093.08	kJ/mol	Joback Method
hf	-1613.41	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	95.83	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.298		Crippen Method
mcvol	273.500	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1931.30		NIST Webbook
rinpol	1931.30		NIST Webbook
tb	945.61	K	Joback Method
tc	1159.15	K	Joback Method
tf	585.88	K	Joback Method
vc	1.034	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.78	J/molxK	945.61	Joback Method
cpg	879.15	J/molxK	981.20	Joback Method
cpg	887.94	J/molxK	1016.79	Joback Method
cpg	895.11	J/molxK	1052.38	Joback Method
cpg	900.62	J/molxK	1087.97	Joback Method
cpg	904.43	J/molxK	1123.56	Joback Method
cpg	906.51	J/molxK	1159.15	Joback Method
dvisc	0.0002903	Paxs	585.88	Joback Method

dvisc	0.0001597	Paxs	645.84	Joback Method
dvisc	0.0000972	Paxs	705.79	Joback Method
dvisc	0.0000640	Paxs	765.75	Joback Method
dvisc	0.0000448	Paxs	825.70	Joback Method
dvisc	0.0000328	Paxs	885.65	Joback Method
dvisc	0.0000251	Paxs	945.61	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R488827&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R488827&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>dvisc:</b>	Dynamic viscosity
<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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