

# Sorbitol, 2,6-dimethyl, acetylated

**Inchi:** InChI=1S/C16H26O10/c1-9(17)23-8-13(22-6)15(25-11(3)19)16(26-12(4)20)14(7-21-5)24  
**InchiKey:** UZCWYWPMQTQZNMH-FZKQCIBNSA-N  
**Formula:** C16H26O10  
**SMILES:** COCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC  
**Mol. weight [g/mol]:** 378.37

## Physical Properties

Property code	Value	Unit	Source
gf	-1071.60	kJ/mol	Joback Method
hf	-1638.33	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	91.10	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.006		Crippen Method
mcvol	277.800	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	913.72	K	Joback Method
tc	1121.04	K	Joback Method
tf	543.18	K	Joback Method
vc	1.040	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.98	J/molxK	913.72	Joback Method
cpg	898.98	J/molxK	948.27	Joback Method
cpg	909.42	J/molxK	982.83	Joback Method
cpg	918.25	J/molxK	1017.38	Joback Method
cpg	925.43	J/molxK	1051.93	Joback Method
cpg	930.92	J/molxK	1086.48	Joback Method
cpg	934.66	J/molxK	1121.04	Joback Method

dvisc	0.0002856	Paxs	543.18	Joback Method
dvisc	0.0001429	Paxs	604.94	Joback Method
dvisc	0.0000813	Paxs	666.69	Joback Method
dvisc	0.0000508	Paxs	728.45	Joback Method
dvisc	0.0000342	Paxs	790.21	Joback Method
dvisc	0.0000244	Paxs	851.96	Joback Method
dvisc	0.0000182	Paxs	913.72	Joback Method

## Sources

<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=R527690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R527690&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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