

# Sorbitol, 6-methyl, acetylated

**Inchi:** InChI=1S/C17H26O11/c1-9(18)24-8-15(26-11(3)20)17(28-13(5)22)16(27-12(4)21)14(7-2  
**InchiKey:** OFLLMJLGPARRK-QZWWFDLISA-N  
**Formula:** C17H26O11  
**SMILES:** COCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O  
**Mol. weight [g/mol]:** 406.38

## Physical Properties

Property code	Value	Unit	Source
gf	-1192.10	kJ/mol	Joback Method
hf	-1771.55	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	100.07	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	-0.077		Crippen Method
mcvol	293.460	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	990.47	K	Joback Method
tc	1212.63	K	Joback Method
tf	604.38	K	Joback Method
vc	1.101	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.08	J/molxK	990.47	Joback Method
cpg	977.42	J/molxK	1175.61	Joback Method
cpg	976.55	J/molxK	1138.58	Joback Method
cpg	973.52	J/molxK	1101.55	Joback Method
cpg	968.40	J/molxK	1064.52	Joback Method
cpg	961.23	J/molxK	1027.50	Joback Method
cpg	976.08	J/molxK	1212.63	Joback Method

dvisc	0.0000142	Paxs	990.47	Joback Method
dvisc	0.0000189	Paxs	926.12	Joback Method
dvisc	0.0000261	Paxs	861.77	Joback Method
dvisc	0.0000381	Paxs	797.42	Joback Method
dvisc	0.0000593	Paxs	733.08	Joback Method
dvisc	0.0001006	Paxs	668.73	Joback Method
dvisc	0.0001910	Paxs	604.38	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=R527818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R527818&amp;Units=SI</a>
<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>

## 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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