

# 1,5-Anhydro-3-O-acetyl-2,4,6-tri-O-methyl-D-mann

<b>Other names:</b>	3-O-Acetyl-1,5-anhydro-2,4,6-tri-O-methyl-D-mannitol
<b>Inchi:</b>	InChI=1S/C11H20O6/c1-7(12)17-11-8(14-3)6-16-9(5-13-2)10(11)15-4/h8-11H,5-6H2,1-4
<b>InchiKey:</b>	UHHBRTSQTUOMIP-DBIOUOCHSA-N
<b>Formula:</b>	C11H20O6
<b>SMILES:</b>	COCC1OCC(OC)C(OC(C)=O)C1OC
<b>Mol. weight [g/mol]:</b>	248.27
<b>CAS:</b>	93635-89-3

## Physical Properties

Property code	Value	Unit	Source
gf	-591.98	kJ/mol	Joback Method
hf	-1050.53	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	0.02		Crippen Method
logp	-0.007		Crippen Method
mcvol	185.910	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1545.54		NIST Webbook
tb	627.12	K	Joback Method
tc	822.64	K	Joback Method
tf	373.81	K	Joback Method
vc	0.680	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.85	J/molxK	627.12	Joback Method
cpg	543.85	J/molxK	659.71	Joback Method
cpg	561.01	J/molxK	692.29	Joback Method
cpg	577.30	J/molxK	724.88	Joback Method
cpg	592.68	J/molxK	757.46	Joback Method
cpg	607.10	J/molxK	790.05	Joback Method
cpg	620.52	J/molxK	822.64	Joback Method

dvisc	0.0010224	Paxs	373.81	Joback Method
dvisc	0.0006464	Paxs	416.03	Joback Method
dvisc	0.0004447	Paxs	458.25	Joback Method
dvisc	0.0003259	Paxs	500.47	Joback Method
dvisc	0.0002506	Paxs	542.68	Joback Method
dvisc	0.0002002	Paxs	584.90	Joback Method
dvisc	0.0001648	Paxs	627.12	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=C93635893&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93635893&amp;Units=SI</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>mvol:</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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