

# 2,4-Di-O-acetyl-1,5-anhydro-3,6-di-O-methyl-D-glucopyranose

<b>Inchi:</b>	InChI=1S/C12H20O7/c1-7(13)18-10-6-17-9(5-15-3)12(11(10)16-4)19-8(2)14/h9-12H,5-6H
<b>InchiKey:</b>	NLSNAZMVLFEFGP-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O7
<b>SMILES:</b>	COCC1OCC(OC(C)=O)C(OC)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	276.28

## Physical Properties

Property code	Value	Unit	Source
gf	-712.48	kJ/mol	Joback Method
hf	-1183.75	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	-0.090		Crippen Method
mcvol	201.570	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1694.42		NIST Webbook
tb	703.87	K	Joback Method
tc	903.99	K	Joback Method
tf	435.01	K	Joback Method
vc	0.743	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.82	J/molxK	703.87	Joback Method
cpg	620.83	J/molxK	737.22	Joback Method
cpg	636.79	J/molxK	770.58	Joback Method
cpg	651.67	J/molxK	803.93	Joback Method
cpg	665.42	J/molxK	837.28	Joback Method
cpg	678.02	J/molxK	870.64	Joback Method
cpg	689.40	J/molxK	903.99	Joback Method
dvisc	0.0009285	Paxs	435.01	Joback Method
dvisc	0.0006006	Paxs	479.82	Joback Method

dvisc	0.0004185	Paxs	524.63	Joback Method
dvisc	0.0003087	Paxs	569.44	Joback Method
dvisc	0.0002380	Paxs	614.25	Joback Method
dvisc	0.0001902	Paxs	659.06	Joback Method
dvisc	0.0001563	Paxs	703.87	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357214&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357214&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>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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