

# 2,4-Dimethyl-1,3,6-triacetylglucoside (A)

<b>Inchi:</b>	InChI=1S/C14H22O9/c1-7(15)20-6-10-11(18-4)12(21-8(2)16)13(19-5)14(23-10)22-9(3)17
<b>InchiKey:</b>	MBLDITUADYHZHF-ARDLJMPDSA-N
<b>Formula:</b>	C14H22O9
<b>SMILES:</b>	COC1C(COC(C)=O)OC(OC(C)=O)C(OC)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	334.32

## Physical Properties

Property code	Value	Unit	Source
gf	-937.27	kJ/mol	Joback Method
hf	-1490.17	kJ/mol	Joback Method
hfus	46.85	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	-0.201		Crippen Method
mcvol	237.190	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	821.25	K	Joback Method
tc	1024.83	K	Joback Method
tf	525.47	K	Joback Method
vc	0.877	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.99	J/molxK	821.25	Joback Method
cpg	830.24	J/molxK	990.90	Joback Method
cpg	821.15	J/molxK	956.97	Joback Method
cpg	810.41	J/molxK	923.04	Joback Method
cpg	798.10	J/molxK	889.11	Joback Method
cpg	784.28	J/molxK	855.18	Joback Method
cpg	837.63	J/molxK	1024.83	Joback Method

dvisc	0.0001216	Paxs	821.25	Joback Method
dvisc	0.0001458	Paxs	771.95	Joback Method
dvisc	0.0001793	Paxs	722.66	Joback Method
dvisc	0.0002272	Paxs	673.36	Joback Method
dvisc	0.0002989	Paxs	624.06	Joback Method
dvisc	0.0004122	Paxs	574.77	Joback Method
dvisc	0.0006037	Paxs	525.47	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=R117505&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R117505&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>

## 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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