

# 2,3,6-Tri-O-Acetyl-1,5-Anhydro-4-O-methyl-D-gala

<b>Inchi:</b>	InChI=1S/C13H20O8/c1-7(14)18-5-10-12(17-4)13(21-9(3)16)11(6-19-10)20-8(2)15/h10-1
<b>InchiKey:</b>	ZHUADJSMXLMTKC-VOAKCMCISA-N
<b>Formula:</b>	C13H20O8
<b>SMILES:</b>	COC1C(COC(C)=O)OCC(OC(C)=O)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	304.29

## Physical Properties

Property code	Value	Unit	Source
gf	-832.98	kJ/mol	Joback Method
hf	-1316.97	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	78.42	kJ/mol	Joback Method
log10ws	-0.37		Crippen Method
logp	-0.173		Crippen Method
mcvol	217.230	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinsol	1850.75		NIST Webbook
tb	780.62	K	Joback Method
tc	985.59	K	Joback Method
tf	496.21	K	Joback Method
vc	0.804	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.74	J/molxK	780.62	Joback Method
cpg	743.76	J/molxK	951.43	Joback Method
cpg	733.66	J/molxK	917.27	Joback Method
cpg	722.16	J/molxK	883.11	Joback Method
cpg	709.31	J/molxK	848.94	Joback Method
cpg	695.16	J/molxK	814.78	Joback Method
cpg	752.43	J/molxK	985.59	Joback Method
dvisc	0.0001413	Paxs	780.62	Joback Method
dvisc	0.0001719	Paxs	733.22	Joback Method

dvisc	0.0002150	Paxs	685.82	Joback Method
dvisc	0.0002778	Paxs	638.41	Joback Method
dvisc	0.0003742	Paxs	591.01	Joback Method
dvisc	0.0005308	Paxs	543.61	Joback Method
dvisc	0.0008049	Paxs	496.21	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=R179756&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R179756&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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