

# 4-O-acetyl-1,5-Anhydro-2,3-di-O-methyl-D-ribitol

<b>Inchi:</b>	InChI=1S/C9H16O5/c1-6(10)14-8-5-13-4-7(11-2)9(8)12-3/h7-9H,4-5H2,1-3H3/t7-,8+,9-/m
<b>InchiKey:</b>	NFTACBULRBCFQP-HRDYMLBCSA-N
<b>Formula:</b>	C9H16O5
<b>SMILES:</b>	COC1COCC(OC(C)=O)C1OC
<b>Mol. weight [g/mol]:</b>	204.22

## Physical Properties

Property code	Value	Unit	Source
gf	-496.11	kJ/mol	Joback Method
hf	-856.69	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.022		Crippen Method
mcvol	151.860	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpola	1344.54		NIST Webbook
tb	563.61	K	Joback Method
tc	766.45	K	Joback Method
tf	333.28	K	Joback Method
vc	0.551	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.65	J/molxK	563.61	Joback Method
cpg	411.26	J/molxK	597.42	Joback Method
cpg	427.15	J/molxK	631.22	Joback Method
cpg	442.31	J/molxK	665.03	Joback Method
cpg	456.70	J/molxK	698.84	Joback Method
cpg	470.29	J/molxK	732.64	Joback Method
cpg	483.06	J/molxK	766.45	Joback Method
dvisc	0.0015574	Paxs	333.28	Joback Method
dvisc	0.0009409	Paxs	371.67	Joback Method

dvisc	0.0006247	Paxs	410.06	Joback Method
dvisc	0.0004449	Paxs	448.44	Joback Method
dvisc	0.0003342	Paxs	486.83	Joback Method
dvisc	0.0002618	Paxs	525.22	Joback Method
dvisc	0.0002121	Paxs	563.61	Joback Method

## Sources

<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=R194646&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R194646&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>mccvol:</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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