

# 1,6-Anhydro-2,3-O-isopropylidene-«beta»-D-mann

<b>Inchi:</b>	InChI=1S/C9H14O5/c1-9(2)13-6-5(10)4-3-11-8(12-4)7(6)14-9/h4-8,10H,3H2,1-2H3
<b>InchiKey:</b>	VEESJHGZLRXGHP-UHFFFAOYSA-N
<b>Formula:</b>	C9H14O5
<b>SMILES:</b>	CC1(C)OC2C3OCC(O3)C(O)C2O1
<b>Mol. weight [g/mol]:</b>	202.20
<b>CAS:</b>	14440-51-8

## Physical Properties

Property code	Value	Unit	Source
gf	-326.97	kJ/mol	Joback Method
hf	-749.02	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	-0.378		Crippen Method
mcvol	134.440	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1436.60		NIST Webbook
tb	620.29	K	Joback Method
tc	831.31	K	Joback Method
tf	416.25	K	Joback Method
vc	0.492	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.87	J/molxK	620.29	Joback Method
cpg	433.31	J/molxK	655.46	Joback Method
cpg	446.90	J/molxK	690.63	Joback Method
cpg	459.76	J/molxK	725.80	Joback Method
cpg	472.03	J/molxK	760.97	Joback Method
cpg	483.85	J/molxK	796.14	Joback Method
cpg	495.36	J/molxK	831.31	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=C14440518&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14440518&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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