

# D-Mannaric acid, 1,4:3,6-dilactone

<b>Inchi:</b>	InChI=1S/C6H6O6/c7-1-3-4(12-5(1)9)2(8)6(10)11-3/h1-4,7-8H
<b>InchiKey:</b>	QRFNDAVXJCGLFB-UHFFFAOYSA-N
<b>Formula:</b>	C6H6O6
<b>SMILES:</b>	O=C1OC2C(O)C(=O)OC2C1O
<b>Mol. weight [g/mol]:</b>	174.11
<b>CAS:</b>	2900-01-8

## Physical Properties

Property code	Value	Unit	Source
chs	-2153.40 ± 2.60	kJ/mol	NIST Webbook
gf	-609.54	kJ/mol	Joback Method
hf	-918.43	kJ/mol	Joback Method
hfus	28.66	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Joback Method
log10ws	1.18		Crippen Method
logp	-2.441		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
tb	723.26	K	Joback Method
tc	935.55	K	Joback Method
tf	488.96	K	Joback Method
vc	0.361	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.26	J/mol×K	723.26	Joback Method
cpg	333.81	J/mol×K	758.64	Joback Method
cpg	342.69	J/mol×K	794.02	Joback Method
cpg	350.87	J/mol×K	829.41	Joback Method
cpg	358.34	J/mol×K	864.79	Joback Method
cpg	365.06	J/mol×K	900.17	Joback Method
cpg	371.03	J/mol×K	935.55	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=C2900018&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2900018&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>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>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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