

# 1,2,3-Cyclohexanetriol

Inchi:	InChI=1S/C6H12O3/c7-4-2-1-3-5(8)6(4)9/h4-9H,1-3H2
InchiKey:	IZSANPWSFUSNMY-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	OC1CCCC(O)C1O
Mol. weight [g/mol]:	132.16
CAS:	6286-43-7

## Physical Properties

Property code	Value	Unit	Source
gf	-401.79	kJ/mol	Joback Method
hf	-610.22	kJ/mol	Joback Method
hfus	17.54	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	-0.747		Crippen Method
mcvol	102.150	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
tb	623.43	K	Joback Method
tc	799.96	K	Joback Method
tf	340.15 ± 2.00	K	NIST Webbook
vc	0.359	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.87	J/mol×K	623.43	Joback Method
cpg	337.02	J/mol×K	770.54	Joback Method
cpg	329.13	J/mol×K	741.12	Joback Method
cpg	320.78	J/mol×K	711.70	Joback Method
cpg	311.96	J/mol×K	682.27	Joback Method
cpg	302.66	J/mol×K	652.85	Joback Method
cpg	344.44	J/mol×K	799.96	Joback Method
dvisc	0.0000159	Paxs	623.43	Joback Method
dvisc	0.0000337	Paxs	575.98	Joback Method

dvisc	0.0000815	Paxs	528.53	Joback Method
dvisc	0.0002344	Paxs	481.09	Joback Method
dvisc	0.0008498	Paxs	433.64	Joback Method
dvisc	0.0042281	Paxs	386.19	Joback Method
dvisc	0.0329758	Paxs	338.74	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6286437&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6286437&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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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