

# 1,3,4,5-Tetrahydrocyclohexanecarboxylic acid, gamma-lactone

Inchi:	InChI=1S/C7H10O5/c8-3-1-7(11)2-4(5(3)9)12-6(7)10/h3-5,8-9,11H,1-2H2
InchiKey:	QPJRIFFWEBJVFN-UHFFFAOYSA-N
Formula:	C7H10O5
SMILES:	O=C1OC2CC1(O)CC(O)C2O
Mol. weight [g/mol]:	174.15
CAS:	640-06-2

## Physical Properties

Property code	Value	Unit	Source
gf	-534.72	kJ/mol	Joback Method
hf	-806.36	kJ/mol	Joback Method
hfus	21.55	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	0.36		Crippen Method
logp	-1.841		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	5926.27	kPa	Joback Method
tb	743.79	K	Joback Method
tc	940.53	K	Joback Method
tf	490.16	K	Joback Method
vc	0.406	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.39	J/molxK	743.79	Joback Method
cpg	377.78	J/molxK	776.58	Joback Method
cpg	386.91	J/molxK	809.37	Joback Method
cpg	395.86	J/molxK	842.16	Joback Method
cpg	404.71	J/molxK	874.95	Joback Method
cpg	413.52	J/molxK	907.74	Joback Method
cpg	422.38	J/molxK	940.53	Joback Method

# Sources

<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=C640062&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C640062&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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