

# Tricarballylic acid

<b>Other names:</b>	1,2,3-Propanetricarboxylic acid «beta»-Carboxyglutaric acid Carballylic acid Propane 1,2,3-tricarboxylic acid Tricarballylate
<b>Inchi:</b>	InChI=1S/C6H8O6/c7-4(8)1-3(6(11)12)2-5(9)10/h3H,1-2H2,(H,7,8)(H,9,10)(H,11,12)
<b>InchiKey:</b>	KQTIICEAUMSDG-UHFFFAOYSA-N
<b>Formula:</b>	C6H8O6
<b>SMILES:</b>	O=C(O)CC(CC(=O)O)C(=O)O
<b>Mol. weight [g/mol]:</b>	176.12
<b>CAS:</b>	99-14-9

## Physical Properties

Property code	Value	Unit	Source
gf	-800.02	kJ/mol	Joback Method
hf	-966.88	kJ/mol	Joback Method
hfus	24.83	kJ/mol	Joback Method
hvap	98.84	kJ/mol	Joback Method
log10ws	0.61		Crippen Method
logp	-0.363		Crippen Method
mcvol	117.720	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
tb	774.39	K	Joback Method
tc	958.00	K	Joback Method
tf	474.63	K	Joback Method
vc	0.441	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.91	J/molxK	774.39	Joback Method
cpg	326.27	J/molxK	804.99	Joback Method
cpg	331.27	J/molxK	835.59	Joback Method
cpg	335.93	J/molxK	866.19	Joback Method

cpg	340.25	J/molxK	896.80	Joback Method
cpg	344.25	J/molxK	927.40	Joback Method
cpg	347.93	J/molxK	958.00	Joback Method
dvisc	0.0008139	Paxs	474.63	Joback Method
dvisc	0.0002075	Paxs	524.59	Joback Method
dvisc	0.0000671	Paxs	574.55	Joback Method
dvisc	0.0000260	Paxs	624.51	Joback Method
dvisc	0.0000116	Paxs	674.47	Joback Method
dvisc	0.0000058	Paxs	724.43	Joback Method
dvisc	0.0000032	Paxs	774.39	Joback Method

## Sources

<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=C99149&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C99149&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>

## 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>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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