

# Triethyl citrate

Other names:	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-triethyl ester
	1,2,3-propanetricarboxylic acid, 2-hydroxy-, triethyl ester
	2-Hydroxy-1,2,3-propanetricarboxylic acid, triethyl ester
	Citroflex 2
	Crodamol TC
	Eudraflex
	Hydagen C.A.T
	Hydragen CAT
	NSC 8907
	TEC
	Triethyl 2-hydroxy-1,2,3-propanetricarboxylate
	Triethylester kyseliny citronove
	Uniflex TEC
	Uniplex 80
	citric acid, triethyl ester
Inchi:	InChI=1S/C12H20O7/c1-4-17-9(13)7-12(16,11(15)19-6-3)8-10(14)18-5-2/h16H,4-8H2,1-
InchiKey:	DOOTYTYQINUNNV-UHFFFAOYSA-N
Formula:	C12H20O7
SMILES:	CCOC(=O)CC(O)(CC(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	276.28
CAS:	77-93-0

## Physical Properties

Property code	Value	Unit	Source
dvisc	0.0321000	Paxs	Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents
gf	-785.58	kJ/mol	Joback Method
hf	-1186.39	kJ/mol	Joback Method
hfs	-1492.00	kJ/mol	NIST Webbook
hfus	31.87	kJ/mol	Joback Method
hvap	85.16	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.187		Crippen Method
mcvol	208.130	ml/mol	McGowan Method

pc	2222.89	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1659.40		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1659.40		NIST Webbook
rinpol	1659.00		NIST Webbook
ripol	2461.00		NIST Webbook
ripol	2461.00		NIST Webbook
tb	567.20	K	NIST Webbook
tc	981.50	K	Joback Method
tf	504.72	K	Joback Method
vc	0.787	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.32	J/molxK	918.26	Joback Method
cpg	642.51	J/molxK	855.02	Joback Method
cpg	631.95	J/molxK	823.40	Joback Method
cpg	620.61	J/molxK	791.78	Joback Method
cpg	669.58	J/molxK	949.88	Joback Method
cpg	677.08	J/molxK	981.50	Joback Method
cpg	652.30	J/molxK	886.64	Joback Method
dvisc	0.0001961	Paxs	552.56	Joback Method
dvisc	0.0001024	Paxs	600.41	Joback Method
dvisc	0.0000588	Paxs	648.25	Joback Method
dvisc	0.0000365	Paxs	696.09	Joback Method
dvisc	0.0000241	Paxs	743.94	Joback Method
dvisc	0.0000167	Paxs	791.78	Joback Method
dvisc	0.0004247	Paxs	504.72	Joback Method
hvapt	68.20	kJ/mol	473.50	NIST Webbook
rhoI	1097.30	kg/m3	338.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1102.80	kg/m3	333.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties

rhoI	1106.60	kg/m3	328.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1112.10	kg/m3	323.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1116.50	kg/m3	318.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1122.40	kg/m3	313.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1126.20	kg/m3	308.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1131.10	kg/m3	303.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1134.50	kg/m3	298.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhoI	1138.40	kg/m3	293.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.20	K	0.10	NIST Webbook

# Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C77930&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C77930&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Investigation of SO <sub>2</sub> solubilities in some biobased solvents and their thermodynamic properties:	<a href="https://www.doi.org/10.1016/j.jct.2017.12.021">https://www.doi.org/10.1016/j.jct.2017.12.021</a>
Properties of Carbon Dioxide in Some Biobased Solvents:	<a href="https://www.doi.org/10.1021/acs.jced.6b00399">https://www.doi.org/10.1021/acs.jced.6b00399</a>
Synthesis and Characterization of Diethyl Citrate and Phase Equilibria in Mixtures with Ethanol and Water:	<a href="https://www.doi.org/10.1021/acs.jced.7b01060">https://www.doi.org/10.1021/acs.jced.7b01060</a>
Joback Method:	<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>hfs:</b>	Solid phase 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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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