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
	ethyl citrate
Inchi:	InChI=1S/C12H20O7/c1-4-17-9(13)7-12(16,11(15)19-6-3)8-10(14)18-5-2/h16H,4-8H2,1-3
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	Pa×s	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	1659.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1659.40		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1659.40		NIST Webbook
rinpol	1656.00		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	642.51	J/mol×K	855.02	Joback Method
cpg	620.61	J/mol×K	791.78	Joback Method
cpg	652.30	J/mol×K	886.64	Joback Method
cpg	661.32	J/mol×K	918.26	Joback Method
cpg	669.58	J/mol×K	949.88	Joback Method
cpg	677.08	J/mol×K	981.50	Joback Method
cpg	631.95	J/mol×K	823.40	Joback Method
dvisc	0.0001961	Pa×s	552.56	Joback Method
dvisc	0.0001024	Pa×s	600.41	Joback Method
dvisc	0.0000588	Pa×s	648.25	Joback Method
dvisc	0.0000365	Pa×s	696.09	Joback Method
dvisc	0.0000241	Pa×s	743.94	Joback Method
dvisc	0.0004247	Pa×s	504.72	Joback Method
dvisc	0.0000167	Pa×s	791.78	Joback Method
hvapt	68.20	kJ/mol	473.50	NIST Webbook
rhol	1097.30	kg/m3	338.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1102.80	kg/m3	333.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties

rhol	1106.60	kg/m3	328.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1112.10	kg/m3	323.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1122.40	kg/m3	313.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1126.20	kg/m3	308.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1131.10	kg/m3	303.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1134.50	kg/m3	298.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1138.40	kg/m3	293.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1116.50	kg/m3	318.15	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:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties:	https://www.doi.org/10.1016/j.jct.2017.12.021
Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents:	https://www.doi.org/10.1021/acs.jced.6b00399
Synthesis and Characterization of Diethyl Citrate and Phase Equilibria in Mixtures with Ethanol and Water:	https://www.doi.org/10.1021/acs.jced.7b01060
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume