O-Acetylcitric acid triethyl ester

Other names:	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, 1,2,3-triethyl ester
	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, triethyl ester
	1,2,3-Propanetricarboxylic acid, 2-acetoxy-, triethyl ester
	ATEC
	Acetyl triethyl citrate
	Citric acid, acetyl triethyl ester
	Citric acid, triethyl ester, acetate
	Citroflex A 2
	NSC 3887
	Tricarballylic acid, «beta»-acetoxytributyl ester
	Triethyl 2-(acetyloxy)-1,2,3-propanetricarboxylate
	Triethyl 2-acetoxy-1,2,3-propanetricarboxylate
	Triethyl O-acetylcitrate
	Triethyl acetylcitrate
	Triethylester kyseliny acetylcitronove
	Uniplex 82
	triethyl 2-acetoxypropane-1,2,3-tricarboxylate
	triethyl 2-acetyloxy-1,2,3-propanetricarboxylate
	triethyl acetyl citrate
	triethyl citrate acetate
Inchi:	InChI=1S/C14H22O8/c1-5-19-11(16)8-14(22-10(4)15,13(18)21-7-3)9-12(17)20-6-2/h5-9H
InchiKey:	WEAPVABOECTMGR-UHFFFAOYSA-N
Formula:	C14H22O8
SMILES:	CCOC(=O)CC(CC(=O)OCC)(OC(C)=O)C(=O)OCC
Mol. weight [g/mol]:	318.32
CAS:	77-89-4

Physical Properties

Property code	Value	Unit	Source
dvisc	0.0465500	Pa×s	Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents
gf	-865.84	kJ/mol	Joback Method
hf	-1320.24	kJ/mol	Joback Method
hfus	35.75	kJ/mol	Joback Method
hvap	82.09	kJ/mol	Joback Method

log10ws	-1.24		Crippen Method
logp	0.758		Crippen Method
mcvol	237.880	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	821.65	K	Joback Method
tc	1019.88	K	Joback Method
tf	538.60	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.51	J/mol×K	1019.88	Joback Method
cpg	729.91	J/mol×K	854.69	Joback Method
cpg	741.48	J/mol×K	887.73	Joback Method
cpg	752.02	J/mol×K	920.77	Joback Method
cpg	761.55	J/mol×K	953.80	Joback Method
cpg	770.05	J/mol×K	986.84	Joback Method
cpg	717.34	J/mol×K	821.65	Joback Method
dvisc	0.0004345	Pa×s	538.60	Joback Method
dvisc	0.0002636	Pa×s	585.77	Joback Method
dvisc	0.0001723	Pa×s	632.95	Joback Method
dvisc	0.0001194	Pa×s	680.12	Joback Method
dvisc	0.0000868	Pa×s	727.30	Joback Method
dvisc	0.0000512	Pa×s	821.65	Joback Method
dvisc	0.0000656	Pa×s	774.47	Joback Method
rhol	1142.10	kg/m3	293.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1137.50	kg/m3	298.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties

rhol	1133.10	kg/m3	303.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1127.60	kg/m3	308.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1124.10	kg/m3	313.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1118.50	kg/m3	318.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1115.10	kg/m3	323.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1110.10	kg/m3	328.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1105.40	kg/m3	333.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1100.50	kg/m3	338.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77894&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume