Triacetin

Other names:	1,2,3-Propanetriol, 1,2,3-triacetate
	1,2,3-Propanetriol, triacetate
	1,2,3-propanetriol triacetate
	1,2,3-propanetriol triethanoate
	2-(Acetyloxy)-1-[(acetyloxy)methyl]ethyl acetate
	Acetin, tri-
	Enzactin
	Fungacetin
	Glycerin triacetate
	Glycerol triacetate
	Glycerol, acetylated
	Glyceryl triacetate
	Glyped
	Kesscoflex TRA
	Kodaflex triacetin
	NSC 4796
	Triacetine
	Triacetyl glycerin
	Triacetyl glycerine
	Triacetyl glycerol
	Vanay
	glyceryl triethanoate
Inchi:	InChI=1S/C9H14O6/c1-6(10)13-4-9(15-8(3)12)5-14-7(2)11/h9H,4-5H2,1-3H3
InchiKey:	URAYPUMNDPQOKB-UHFFFAOYSA-N
Formula:	C9H14O6
SMILES:	CC(=O)OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]:	218.20
CAS:	102-76-1

Physical Properties

Property code	Value	Unit	Source
chl	-4211.60 ± 4.20	kJ/mol	NIST Webbook
dvisc	0.0163600	Pa×s	Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents
gf	-679.30	kJ/mol	Joback Method

hf	-968.77	kJ/mol	Joback Method
hfl	-1330.80 ± 4.20	kJ/mol	NIST Webbook
hfus	23.90	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-0.60		Estimated Solubility Method
log10ws	-0.60		Aqueous Solubility Prediction Method
logp	0.044		Crippen Method
mcvol	159.990	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1344.40		NIST Webbook
rinpol	1339.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2077.00		NIST Webbook
sl	458.30	J/mol×K	NIST Webbook
tb	633.75	K	Joback Method
tc	825.52	K	Joback Method
tf	195.00 ± 10.00	K	NIST Webbook
tf	276.40 ± 2.00	K	NIST Webbook
tf	277.30 ± 0.50	K	NIST Webbook
tf	277.15 ± 0.80	K	NIST Webbook
tf	213.00 ± 50.00	K	NIST Webbook
tf	294.90	K	Aqueous Solubility Prediction Method
tt	275.25 ± 0.02	K	NIST Webbook
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.09	J/mol×K	825.52	Joback Method
cpg	462.37	J/mol×K	793.56	Joback Method
cpg	453.02	J/mol×K	761.60	Joback Method
cpg	443.06	J/mol×K	729.63	Joback Method
cpg	432.51	J/mol×K	697.67	Joback Method
cpg	421.38	J/mol×K	665.71	Joback Method
cpg	409.69	J/mol×K	633.75	Joback Method
cpl	384.70	J/mol×K	300.00	NIST Webbook
cpl	402.00	J/mol×K	298.15	NIST Webbook
cpl	389.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0008437	Pa×s	432.85	Joback Method
dvisc	0.0005372	Pa×s	473.03	Joback Method
dvisc	0.0003671	Pa×s	513.21	Joback Method
dvisc	0.0002651	Pa×s	553.39	Joback Method
dvisc	0.0002001	Pa×s	593.57	Joback Method
dvisc	0.0001565	Pa×s	633.75	Joback Method
dvisc	0.0014534	Pa×s	392.67	Joback Method
hfust	25.80	kJ/mol	275.25	NIST Webbook
hfust	25.80	kJ/mol	275.30	NIST Webbook
hfust	25.80	kJ/mol	275.30	NIST Webbook
hvapt	82.00	kJ/mol	301.50	NIST Webbook
rhol	1136.60	kg/m3	313.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1109.40	kg/m3	338.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1114.80	kg/m3	333.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1120.20	kg/m3	328.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties

rhol	1125.70	kg/m3	323.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1142.00	kg/m3	308.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1147.40	kg/m3	303.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1152.90	kg/m3	298.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1158.30	kg/m3	293.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
rhol	1131.10	kg/m3	318.15	Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties
sfust	93.80	J/mol×K	275.25	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58272e+01
Coeff. B	-4.97924e+03
Coeff. C	-8.79290e+01
Temperature range (K), min.	408.35
Temperature range (K), max.	561.43

Sources

Solubilities and Thermodynamic Properties of Carbon Dioxide in Some Biobased Solvents:	https://www.doi.org/10.1021/acs.jced.6b00399
Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties:	https://www.doi.org/10.1016/j.jct.2017.12.021
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102761&Units=SI
Experimental measurement and modeling of the Type 3 ternary system containing (decane + water + triacetin):	https://www.doi.org/10.1016/j.jct.2013.07.009
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-Liquid-Supercritical Fluid Equilibria for Systems Containing Carbon Dioxide, Propane, and Triglycerides:	https://www.doi.org/10.1021/je800995r
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Experimental measurement and prediction of (liquid + liquid + liquid) equilibrium for the system (1-hexadecane + water + triacetin):	https://www.doi.org/10.1016/j.jct.2015.11.011
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous/Organic System. Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume