GLYCEROL TRICAPRYLATE

Other names: 1,2,3-propanetriol trioctanoate
Caprylic acid triglyceride
Caprylic triglyceride
Caprylin
Captex 8000
Emalex KTG
Glycerin tricaprylate
Glycerol trioctanoate
Maceight
Miglyol 808
NSC 4059
Octanoic acid triglyceride
Octanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester
Octanoic acid, 1,2,3-propanetriyl ester
Octanoin, tri-
Panacete 800
RATO
Sefsol 810
Tricaprylic Glyceride
Tricapryloylglycerol
Tricaprylyl glycerin
Trioctanoylglycerol
glyceryl tricaprylate
glyceryl trioctanoate
tricaprilin
tricaprylin
trioctanoin

Inchi: InChI=1S/C27H50O6/c1-4-7-10-13-16-19-25(28)31-22-24(33-27(30)21-18-15-12-9-6-3)2

InchiKey: VLPFTAMPNXLGLX-UHFFFAOYSA-N

Formula: C27H50O6

SMILES: CCCCCCCC(=O)OCC(COC(=O)CCCCCCC)OC(=O)CCCCCCC

Mol. weight [g/mol]: 470.69

Physical Properties

Property code	Value	Unit	Source
chs	-15259.00 ± 1.80	kJ/mol	NIST Webbook

hf	-1516.05	kJ/mol	Cheméo Relay (1.0)
hfus	70.52	kJ/mol	Joback Method
hvap	135.40 ± 4.70	kJ/mol	NIST Webbook
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-6.52		Cheméo Relay (1.0)
logp	7.066		Crippen Method
mcvol	413.610	ml/mol	McGowan Method
pc	744.88	kPa	Joback Method
rinpol	2958.00		NIST Webbook
tb	670.51	K	Cheméo Relay (1.0)
tc	836.00	K	Critical properties, heat capacities, and thermal diffusivities of four saturated triglycerides
tf	294.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.42	J/mol×K	1045.59	Joback Method
cpg	1477.45	J/mol×K	1088.41	Joback Method
cpg	1494.01	J/mol×K	1131.24	Joback Method
cpg	1508.15	J/mol×K	1174.06	Joback Method
cpg	1519.94	J/mol×K	1216.88	Joback Method
cpg	1529.42	J/mol×K	1259.70	Joback Method
cpg	1536.66	J/mol×K	1302.53	Joback Method
cpl	920.00	J/mol×K	338.00	NIST Webbook
dvisc	0.0000964	Pa×s	670.54	Joback Method
dvisc	0.0000529	Pa×s	745.55	Joback Method
dvisc	0.0000324	Pa×s	820.56	Joback Method
dvisc	0.0000216	Pa×s	895.57	Joback Method
dvisc	0.0000153	Pa×s	970.58	Joback Method
dvisc	0.0000114	Pa×s	1045.59	Joback Method
dvisc	0.0002041	Pa×s	595.53	Joback Method
hvapt	118.70	kJ/mol	386.00	NIST Webbook
hvapt	116.00	kJ/mol	424.50	NIST Webbook

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	102.00	952.7
298.15	102.00	948.9
303.15	102.00	944.9
313.15	102.00	937.4
333.15	102.00	922.5
353.15	102.00	907.7
298.15	120.00	949.9
298.15	9830.00	955.5
298.15	20100.00	961.3
298.15	30020.00	966.6
298.15	40050.00	971.9
298.15	50040.00	977.1

Reference *https://www.doi.org/10.1021/acs.jced.8b01046*

Sources

Cheméo Relay (1.0):

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Physical properties of systems of interest to the edible oil industry: https://www.doi.org/10.1016/j.jct.2017.06.012

Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent): https://www.doi.org/10.1021/acs.jced.8b01046

Thermodynamic Modeling of Triglycerides using PC-SAFT: Viscosities of Fatty Mixtures: https://www.doi.org/10.1021/je700293s

Experimental Data and Prediction:

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

Critical properties, heat capacities, and thermal diffusivities of four saturated triglycerides: https://www.doi.org/10.1016/j.jct.2017.07.006

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C538238&Units=SI

Cheméo Relay (1.0, beta):

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
hf:	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
ie:	Ionization energy
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