

Trimyristin

Other names:	1,2,3-propanetriyl tri(tetradecanoate) 2,3-Bis(tetradecanoyloxy)propyl myristate Glyceryl tritetradecanoate Myristin NSC 4062 Tetradecanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester VP 114 dynasan 114 glycerin trimyrystate glycerol trimyrystate glyceryl trimyrystate myristic acid triglyceride myristic triglyceride myristin, tri- tetradecanoic acid 1,2,3-propanetriyl ester tetradecanoic acid, 1,2,3-propanetriyl ester
Inchi:	InChI=1S/C45H86O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-43(46)49-40-42(51-45(48)3
InchiKey:	DUXYWXYOBMKGIN-UHFFFAOYSA-N
Formula:	C45H86O6
SMILES:	CCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCC)OC(=O)CCCCCCCCC
Mol. weight [g/mol]:	723.16
CAS:	555-45-3

Physical Properties

Property code	Value	Unit	Source
chs	-27643.70 ± 1.80	kJ/mol	NIST Webbook
gf	-376.18	kJ/mol	Joback Method
hf	-1711.81	kJ/mol	Joback Method
hfus	117.14	kJ/mol	Joback Method
hvap	199.20 ± 6.90	kJ/mol	NIST Webbook
log10ws	-15.36		Crippen Method
logp	14.088		Crippen Method
mcvol	667.230	ml/mol	McGowan Method
pc	343.95	kPa	Joback Method
sl	1246.00	J/molxK	NIST Webbook
tb	1457.43	K	Joback Method

tc	925.00	K	Critical properties, heat capacities, and thermal diffusivities of four saturated triglycerides
tf	331.10	K	Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane
tt	330.20 ± 0.20	K	NIST Webbook
tt	305.10 ± 1.00	K	NIST Webbook
tt	330.80 ± 1.00	K	NIST Webbook
tt	305.50 ± 0.20	K	NIST Webbook
tt	319.70 ± 1.00	K	NIST Webbook
vc	2.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2538.38	J/mol×K	2403.78	Joback Method
cpg	2603.95	J/mol×K	1457.43	Joback Method
cpg	2550.43	J/mol×K	2246.05	Joback Method
cpg	2572.46	J/mol×K	2088.33	Joback Method
cpg	2596.65	J/mol×K	1930.60	Joback Method
cpg	2615.17	J/mol×K	1772.88	Joback Method
cpg	2620.22	J/mol×K	1615.15	Joback Method
cpl	1555.20	J/mol×K	331.50	NIST Webbook
cpl	1481.00	J/mol×K	333.00	NIST Webbook
dvisc	0.0000017	Paxs	1127.91	Joback Method
dvisc	0.0000005	Paxs	1457.43	Joback Method
dvisc	0.0000056	Paxs	908.23	Joback Method
dvisc	0.0000133	Paxs	798.39	Joback Method
dvisc	0.0000007	Paxs	1347.59	Joback Method
dvisc	0.0000011	Paxs	1237.75	Joback Method
dvisc	0.0000028	Paxs	1018.07	Joback Method
hfust	152.20	kJ/mol	330.20	NIST Webbook
hfust	152.20	kJ/mol	330.20	NIST Webbook
hvapt	155.80	kJ/mol	469.00	NIST Webbook
hvapt	147.80	kJ/mol	519.50	NIST Webbook

Sources

Critical properties, heat capacities, and thermal diffusivities of four saturated hydrocarbons	https://www.doi.org/10.1016/j.jct.2017.07.006
Physical properties of systems of interest to the edible oil industry: Solubilities and Fugacity Model Equations for Binary Systems of Hexadecane + Fatty Acid (Solvent)	https://www.doi.org/10.1016/j.jct.2017.06.012
Solubilities of Fatty Acids and Triglycerides in Bromocyclohexane + Fatty Acid (Solvent)	https://www.doi.org/10.1021/je201181k
Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane: Crippen Method	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method	https://www.doi.org/10.1021/acs.jced.6b00355
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	https://www.chemeo.com/doc/models/crippen_log10ws
	https://en.wikipedia.org/wiki/Joback_method
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C555453&Units=SI

Legend

chs:	Standard solid 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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvp:	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
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

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