Tetradecanoic acid, 1,2,3-propanetriyl ester

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 trimyristate
glycerol trimyristate
glyceryl trimyristate
myristic acid triglyceride
myristic triglyceride
myristin, tri-
tetradecanoic acid 1,2,3-propanetriyl ester
trimyristin

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: CCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCC)OC(=O)CCCCCCCCCC

Mol. weight [g/mol]: 723.18

Physical Properties

Property code	Value	Unit	Source
chs	-27643.70 ± 1.80	kJ/mol	NIST Webbook
hf	-1867.44	kJ/mol	Cheméo Relay (1.0)
hfus	117.14	kJ/mol	Joback Method
hvap	199.20 ± 6.90	kJ/mol	NIST Webbook
ie	10.17	eV	Cheméo Relay (1.0)
log10ws	-11.91		Cheméo Relay (1.0)
logp	14.088		Crippen Method
mcvol	667.230	ml/mol	McGowan Method
pc	343.95	kPa	Joback Method
sl	1246.00	J/mol×K	NIST Webbook
tb	785.45	K	Cheméo Relay (1.0)

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	305.50 ± 0.20	K	NIST Webbook
tt	330.20 ± 0.20	K	NIST Webbook
tt	305.50 ± 0.20	K	NIST Webbook
tt	330.80 ± 1.00	K	NIST Webbook
tt	319.70 ± 1.00	K	NIST Webbook
tt	305.10 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

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

Cheméo Relay (1.0, beta):	
Physical properties of systems of interest to the edible oil industry: Viscosities and densities of model systems formed by (triacylglycerol + fatty acid + solvent):	https://www.doi.org/10.1016/j.jct.2017.06.012
Solubilities of Fatty Acids and Triglycerides in 1-Bromopropane: Joback Method:	https://www.doi.org/10.1021/je201181k
	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C555453&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical properties, heat capacities, and thermal diffusivities of four saturated triglycerides:	https://www.doi.org/10.1016/j.jct.2017.07.006
Solid-Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane:	https://www.doi.org/10.1021/acs.jced.6b00355

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
hfust:	Enthalpy of fusion at a given temperature
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
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