Dodecanoic acid, 1,2,3-propanetriyl ester

Other names:	1,2,3-propanetriyl tridodecanoate
	Dodecanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester
	Dodecanoic acid, tri-ester with glycerol
	Dynasan 112
	Glycerin trilaurate
	Glycerol trilaurate
	Glyceryl tridodecanoate
	Glyceryl trilaurate
	Lauric acid triglyceride
	Lauric acid triglycerin ester
	Laurin, tri-
	NSC 4061
	Tridodecanoyl glycerol
	Trilaurin
	Trilauroylglycerol
Inchi:	InChI=1S/C39H74O6/c1-4-7-10-13-16-19-22-25-28-31-37(40)43-34-36(45-39(42)33-30-2
InchiKey:	VMPHSYLJUKZBJJ-UHFFFAOYSA-N
Formula:	C39H74O6
SMILES:	CCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCC)OC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	639.00
CAS:	538-24-9

Physical Properties

Property code	Value	Unit	Source
chs	-23731.60 ± 1.80	kJ/mol	NIST Webbook
chs	-23860.00	kJ/mol	NIST Webbook
gf	-426.70	kJ/mol	Joback Method
hf	-1587.97	kJ/mol	Joback Method
hfus	101.60	kJ/mol	Joback Method
hvap	180.00 ± 6.30	kJ/mol	NIST Webbook
log10ws	-12.85		Crippen Method
logp	11.747		Crippen Method
mcvol	582.690	ml/mol	McGowan Method
pc	431.15	kPa	Joback Method
sl	1071.50	J/mol×K	NIST Webbook
tb	1320.15	K	Joback Method

tc	899.00	K	Critical properties, heat capacities, and thermal diffusivities of four saturated triglycerides
tf	319.50 ± 0.20	K	NIST Webbook
tf	321.90	K	Solid Liquid Equilibria in the Binary Systems of Saturated Fatty Acids or Triglycerides (C12 to C18) + Hexadecane
tt	287.40 ± 1.00	K	NIST Webbook
tt	307.20 ± 1.00	K	NIST Webbook
tt	319.60 ± 1.00	K	NIST Webbook
vc	2.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2256.06	J/mol×K	1606.41	Joback Method
cpg	2245.17	J/mol×K	1415.57	Joback Method
cpg	2255.43	J/mol×K	1510.99	Joback Method
cpg	2213.69	J/mol×K	1892.67	Joback Method
cpg	2233.82	J/mol×K	1797.25	Joback Method
cpg	2248.40	J/mol×K	1701.83	Joback Method
cpg	2223.91	J/mol×K	1320.15	Joback Method
cpl	1355.60	J/mol×K	330.70	NIST Webbook
cpl	1305.00	J/mol×K	323.00	NIST Webbook
dvisc	0.0000078	Pa×s	927.23	Joback Method
dvisc	0.0000046	Pa×s	1025.46	Joback Method
dvisc	0.0000030	Pa×s	1123.69	Joback Method
dvisc	0.0000021	Pa×s	1221.92	Joback Method
dvisc	0.0000015	Pa×s	1320.15	Joback Method
dvisc	0.0000345	Pa×s	730.77	Joback Method
dvisc	0.0000150	Pa×s	829.00	Joback Method
hfust	123.51	kJ/mol	319.50	NIST Webbook
hfust	123.51	kJ/mol	319.50	NIST Webbook
hvapt	137.60	kJ/mol	489.00	NIST Webbook
hvapt	147.10	kJ/mol	438.00	NIST Webbook
rhol	870.40	kg/m3	353.15	Thermodynamic Modeling of Triglycerides using PC-SAFT
rhol	886.90	kg/m3	333.15	Thermodynamic Modeling of Triglycerides using PC-SAFT

rhol	899.60	kg/m3	313.15	Thermodynamic Modeling of Triglycerides using PC-SAFT
rhol	905.10	kg/m3	303.15	Thermodynamic Modeling of Triglycerides using PC-SAFT

Sources

Solubilities of Fatty Acids and Triglycerides in 1-Bromopropane:	https://www.doi.org/10.1021/je201181k
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1138.mol
Physical properties of systems of interest to the edible oil industry: Critical properties, heat capacities, and thermal diffusivities of four saturated fatty acids + solvent):	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/10.1016/j.jct.2017.07.006
Thermodynamic Modeling of Triglycerides using PC-SAFT:	https://www.doi.org/10.1021/acs.jced.8b01046
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C538249&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
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
rhol:	Liquid Density

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