Decanoic acid, 1,2,3-propanetriyl ester

Other names:	1,2,3-propanetriyl tridecanoate
	CAPRIC ACID TRIGLYCERIDE
	CAPRIN
	Capric triglyceride
	Decanoic acid, 1,1',1''-(1,2,3-propanetriyl) ester
	Decanoin, tri-
	Dynasan 110
	Glycerin tridecanoate
	Glycerol tricaprate
	Glycerol tricaprin
	Glycerol tridecanoate
	Glyceryl tricaprate
	Glyceryl tridecanoate
	NSC 147475
	TRIDECANOIN
	Tricapric glyceride
	Tricaprin
	tri-n-Caprin
Inchi:	InChI=1S/C33H62O6/c1-4-7-10-13-16-19-22-25-31(34)37-28-30(39-33(36)27-24-21-18-1
InchiKey:	LADGBHLMCUINGV-UHFFFAOYSA-N
Formula:	C33H62O6
SMILES:	CCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCC)OC(=O)CCCCCCCCC
Mol. weight [g/mol]:	554.84
CAS:	621-71-6

Physical Properties

Property code	Value	Unit	Source
chs	-19861.40 ± 1.80	kJ/mol	NIST Webbook
gf	-477.22	kJ/mol	Joback Method
hf	-1464.13	kJ/mol	Joback Method
hfus	86.06	kJ/mol	Joback Method
hvap	154.60 ± 5.40	kJ/mol	NIST Webbook
log10ws	-10.34		Crippen Method
logp	9.407		Crippen Method
mcvol	498.150	ml/mol	McGowan Method
pc	556.25	kPa	Joback Method
rinpol	3503.90		NIST Webbook

rinpol	3503.90		NIST Webbook
tb	1182.87	K	Joback Method
tc	864.00	K	Critical properties, heat capacities, and thermal diffusivities of four saturated triglycerides
tf	304.15	K	KDB
tt	291.20 ± 1.00	K	NIST Webbook
tt	263.60 ± 1.00	K	NIST Webbook
tt	305.40 ± 1.00	K	NIST Webbook
vc	1.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1878.30	J/mol×K	1305.35	Joback Method
cpg	1841.03	J/mol×K	1182.87	Joback Method
cpg	1889.56	J/mol×K	1366.60	Joback Method
cpg	1896.26	J/mol×K	1427.84	Joback Method
cpg	1898.65	J/mol×K	1489.08	Joback Method
cpg	1897.00	J/mol×K	1550.32	Joback Method
cpg	1862.21	J/mol×K	1244.11	Joback Method
cpl	1109.00	J/mol×K	313.00	NIST Webbook
dvisc	0.0000390	Pa×s	749.77	Joback Method
dvisc	0.0000208	Pa×s	836.39	Joback Method
dvisc	0.0000124	Pa×s	923.01	Joback Method
dvisc	0.0000081	Pa×s	1009.63	Joback Method
dvisc	0.0000057	Pa×s	1096.25	Joback Method
dvisc	0.0000862	Pa×s	663.15	Joback Method
dvisc	0.0000042	Pa×s	1182.87	Joback Method
hvapt	124.60	kJ/mol	461.00	NIST Webbook
hvapt	130.50	kJ/mol	411.00	NIST Webbook
pvap	1.36e-08	kPa	348.50	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	2.90e-08	kPa	353.48	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	5.99e-08	kPa	358.38	Thermodynamic Modeling of Triglycerides using PC-SAFT

pvap	1.20e-07	kPa	363.18	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	2.94e-08	kPa	353.48	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	5.99e-08	kPa	358.38	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	1.19e-07	kPa	363.18	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	2.23e-07	kPa	367.81	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	2.27e-07	kPa	367.80	Thermodynamic Modeling of Triglycerides using PC-SAFT
pvap	1.39e-08	kPa	348.50	Thermodynamic Modeling of Triglycerides using PC-SAFT

Sources

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=C621716&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic Modeling of Triglycerides using PC-SAFT:	https://www.doi.org/10.1021/acs.jced.8b01046
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1137.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume