Chemical Analysis Report

Report 03-2022

Provided by:
PSE for SPEED Company Limited
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Title:
Chemical analysis of glycerol monooleate, glycerol dioleate and glycerol trioleate

Problem description:
As glycerol monooleate, glycerol dioleate and glycerol trioleate are of interest, physical properties necessary for simulations are reported.

Summary:
- The chemicals have been verified to be of low concern of hazards, no indicated hazard is found.
- Glycerol monooleate is used in foods, pharmaceuticals, cosmetics, rust-preventive oils, vinyl light stabilizers, odorless base paints, textile finishing, and flavoring; used as emulsifier for liquid and paste waxes, polishes, and cleaners
- Glycerol dioleate is used as emollients in cosmetics industry and also used as lubricants and lubricant additives.
- Glycerol trioleate is used as lubricant (e.g. for cosmetics, drugs, and textiles), emulsifier (e.g. for water/oil mixtures), intermediate for radioactive iodine derivatives, and plasticizer; and used in sweet almond oil for medicines and cosmetics

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*Blue text represents estimated value from PSEforSPEED in-house property estimation software

Primary properties

Chemical	Unit	Glycerol monooleate	Glycerol dioleate	Glycerol trioleate
CAS no.		25496-72-4	25637-84-7	122-32-7
SMILE		CCCCCCCCC=CCCCCCCCC(=O)OCC(CO)O	CCCCCCCCC=CCCCCCCCC(=O)OCC(COC(=O)CCCCCCCC=CCCCCCCCC)O	CCCCCCCCC=CCCCCCCCC(=O)OCC(COC(=O)CCCCCCC=CCCCCCCCC)OC(=O)CCCCCCCC=C
MW	g/mol	356.54	620.98	885.43
Tm	K	308.15	328.47	241.15
Tb	K	573.41	543.96	505.25
Tc	K	734.03	748.6	646.31
Pc	bar	33.67	30.86	27.95
Vc	cm^3/mol	944.18	1465.94	1479.17
Zc	-	0.209	0.17	0.144
Gf[298K]	kJ/mol	33.91	-24.06	-33.39
Hf[298K]	kJ/mol	-346.04	-165	-163.18
Omega	-	0.99	2.58	1.23
Hv[298K]	kJ/mol	N/A	N/A	303.45
Hv[Tb]	kJ/mol	102.68	133.43	172.08
Hfus	kJ/mol	41.48	66.5	143.21
Vm[298K]	cm^3/mol	371.95	667.33	965.48
Sol.Par.[298K]	MPa½	18.23	16.78	17.92
SurfTens	dyn/cm	22.09	20.11	26.02
HansenD.sol	MPa½	15.3	16.19	16.96
HansenP.sol	MPa½	3.5	6.47	7.45
HansenH.sol	MPa½	8.07	5.47	7.38
Log(Kow)	-	5.66	13.15	21.11
Log(Ws)	Log(mg/L)	-0.01	-1.13	0.42
pKa	-	10.25	8.38	6.66
AiT	K	559.89	522.64	618.08
Fp	K	445.67	487.66	438.45
Viscosity	cp	N/A	N/A	97.25
THERM.COND	mW/m-K	N/A	N/A	243.42

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Chemical	Unit	Glycerol monooleate	Glycerol dioleate	Glycerol trioleate
CAS no.		25496-72-4	25637-84-7	122-32-7
-Log(LC50)FM	Log(mol/L)	3.74	4.17	3.91
-Log(LC50)DM	Log(mol/L)	N/A	N/A	10.15
-Log(LD50)	Log(mol/kg)	2.84	3.72	4.47
Log(BCF)	-	1	1.16	1.67
-Log(PEL)	Log(mol/m3)	4.74	5.04	5.03
-Log(PCO)	-	0.62	0.57	0.31
Log(GWP)	-	N/A	N/A	N/A
Log(ODP)	-	N/A	N/A	N/A
Log(AP)	-	N/A	N/A	N/A
-LOG(EUAC)	Log(cas/kg)	N/A	N/A	5.82
-LOG(EUANonC)	Log(cas/kg)	N/A	N/A	4.79
-LOG(ERAC)	Log(cas/kg)	N/A	N/A	7.72
-LOG(ERANonC)	Log(cas/kg)	N/A	N/A	5.55
-LOG(EFWC)	Log(cas/kg)	N/A	N/A	4.26
-LOG(EFWNonC)	Log(cas/kg)	N/A	N/A	6.12
-LOG(ESWC)	Log(cas/kg)	N/A	N/A	2.64
-LOG(ESWNonC)	Log(cas/kg)	N/A	N/A	9.12
-LOG(ENSC)	Log(cas/kg)	N/A	N/A	11.19
-LOG(ENSNonC)	Log(cas/kg)	N/A	N/A	14.62
-LOG(EASC)	Log(cas/kg)	N/A	N/A	8.56
-LOG(EASNonC)	Log(cas/kg)	N/A	N/A	10.21
Secondary properties				
Zc	-	0.22	0.144	0.107
Sfus	J/(mol*K)	173.15	263.4	593.87
Vm[Tb]	cm^3/mol	512.71	938.82	1370.68
Refractive Index	-	1.4626	1.04	1.46
Molar Refraction	-	N/A	N/A	263.01
Closed Flash Temp.	K	547.31	594.77	634.69
Open Flash Temp.	K	578.94	665.9	748.18
Dipolar moment	debye	N/A	N/A	0.73
Dielectric const.	-	N/A	N/A	4.09

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Physical properties

Chemical	Unit	Glycerol monooleate	Glycerol dioleate	Glycerol trioleate
CAS no.		25496-72-4	25637-84-7	122-32-7
Henry[298K]	bar*m³/mol	N/A	N/A	1.84E+13
McGowan Volume	cm³/mol	321.63	572.52	823.41

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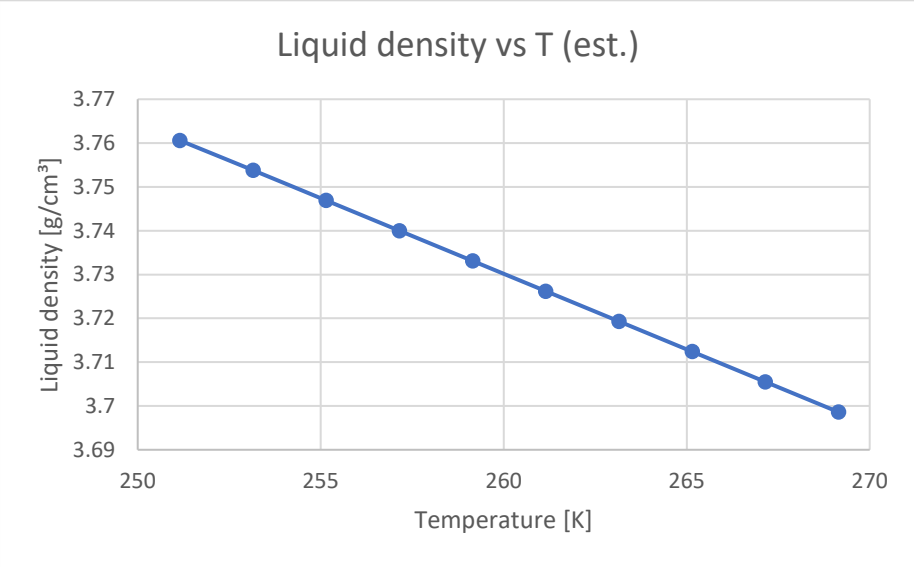
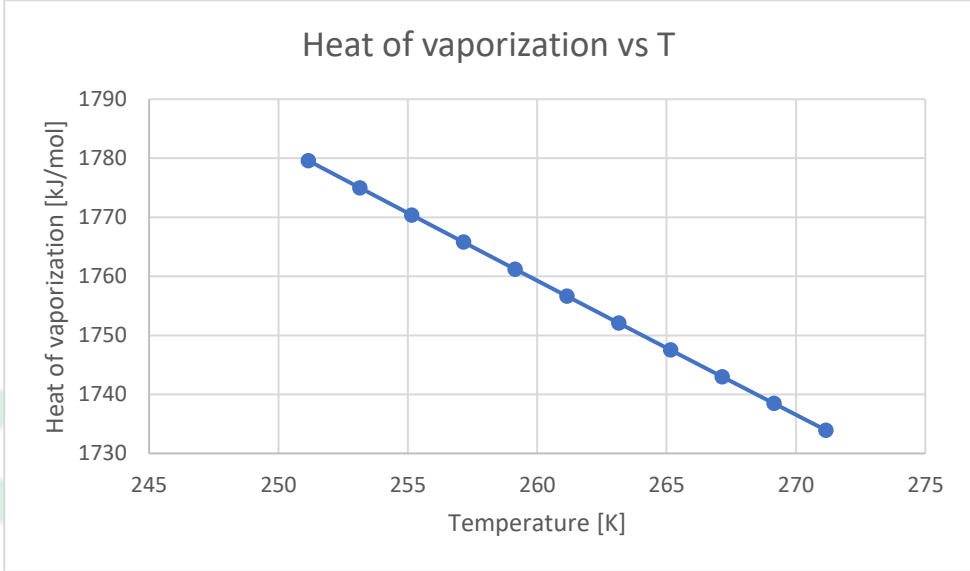
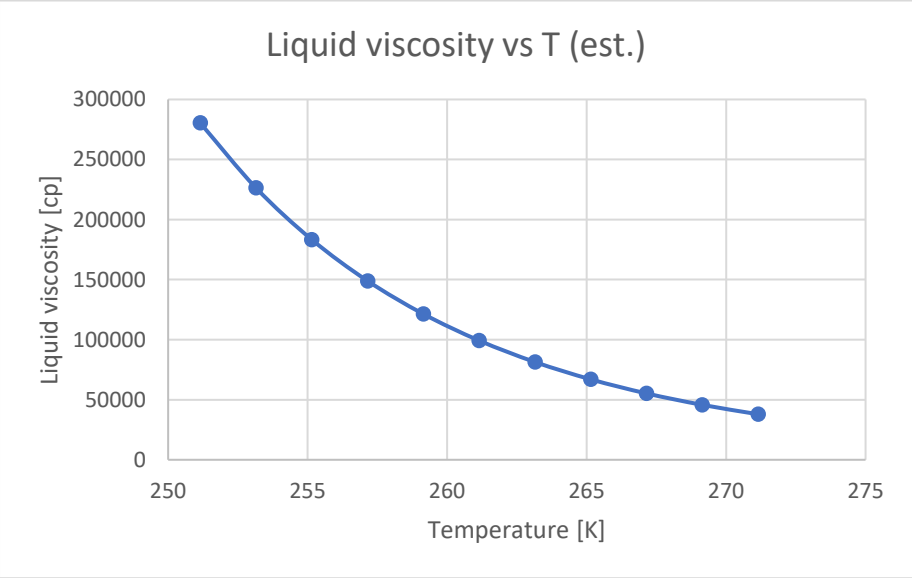
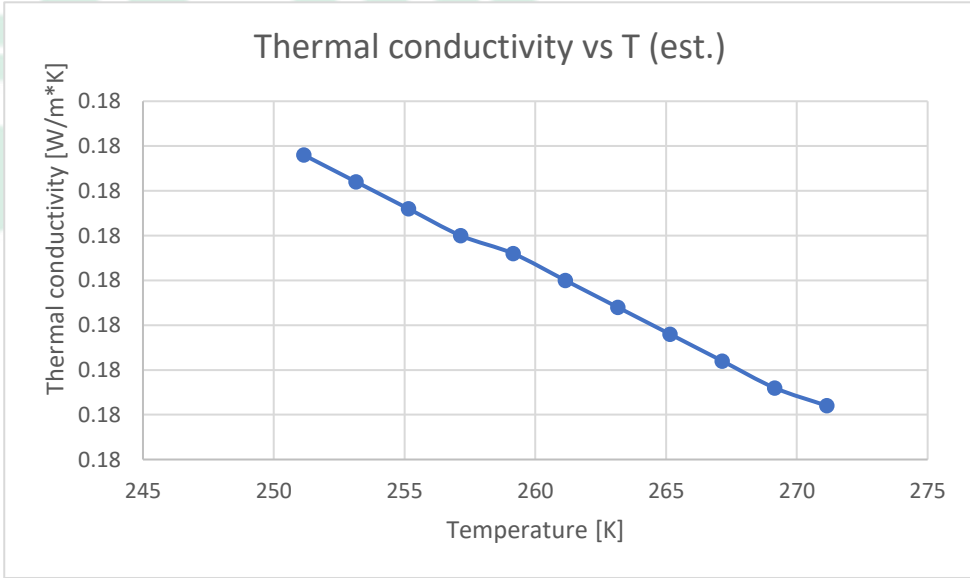
Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

Chemical Glycerol Trioleate









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