Chemical Analysis Report

Report 04-2022

Provided by:
PSE for SPEED Company Limited
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Title:
Chemical analysis of production of acetic acid

Problem description:
Product and alternative raw materials for acetic acid production including acetic acid, ethylene, acetic anhydride and ethyl alcohol are analyzed.

Summary:
- With respect to health hazards, acetic anhydride is the most dangerous and ethylene is the least dangerous.
- Acetic anhydride appears in the list of banned chemicals, so, it is not sure if production of acetic acid through this route would be feasible.
- All are reported under physical hazards, with ethylene and ethyl alcohol as the most dangerous, others have caution; ethylene is also listed as compressed gas.
- In terms of environmental hazards, ethyl alcohol is listed as the most problematic.
- Depending on the conversion, reaction conditions, etc., the choice would be between oxidation of ethylene (could be an option if excess ethylene is available), or, oxidation of ethanol (but it is a two-step reaction, ethanol to acetaldehyde and then to acetic acid, thus increasing the cost);
- Acetic acid, ethanol and ethylene are classified as "good" chemicals because of their many favorable properties, but they need to be used with caution and operations need to be carefully monitored.

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

Primary properties

Chemical	Unit	Acetic acid	Ethylene	Acetic anhydride	Ethyl alcohol
CAS no.		64-19-7	74-85-1	108-24-7	64-17-5
SMILE		O=C(O)C	C=C	O=C(C)OC(=O)C	OCC
MW	g/mol	60.05	28.05	102.09	46.07
Tm	K	289.75	104.15	200.15	159.05
Tb	K	391.05	169.45	412.65	351.35
Tc	K	591.95	282.34	606	513.92
Pc	bar	57.85	50.40	40	61.47
Vc	cm³/mol	179.7	131	290	167
Zc	-	0.277	0.281	0.268	0.277
Gf[298K]	kJ/mol	-374.6	68.44	-473.4	-167.85
Hf[298K]	kJ/mol	-432.8	52.51	-572.5	-234.95
Omega	-	0.47	0.0865	0.45	0.63
Hv[298K]	kJ/mol	23.36	N/A	44.84	42.32
Hv[Tb]	kJ/mol	37.21	N/A	38.36	36.31
Hfus	kJ/mol	11.73	3.35	10.5	4.93
Vm[298K]	cm³/mol	64.47	N/A	92.91	61
Sol.Par.[298K]	MPa½	19.01	12.44	22.01	26.13
SurfTens	dyn/cm	27.1	16	31.93	21.97
HansenD.sol	MPa½	14.5	N/A	16	15.8
HansenP.sol	MPa½	8	N/A	11.7	8.8
HansenH.sol	MPa½	13.5	N/A	10.2	19.4
Log(Kow)	-	-0.17	1.13	-0.67	-0.31
Log(Ws)	Log(mg/L)	6	N/A	5.24	6
pKa	-	4.76	N/A	N/A	15.9
AiT	K	789.26	723.15	603.15	635.93
Fp	K	313.15	494.26	322.59	285.93
Viscosity	cp	1.056	0.01	0.843	4.72
THERM.COND	mW/m-K	159.8	N/A	165.35	165
-Log(LC50)FM	Log(mol/L)	2.86	N/A	3.06	0.52

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Chemical	Unit	Acetic acid	Ethylene	Acetic anhydride	Ethyl alcohol
CAS no.		64-19-7	74-85-1	108-24-7	64-17-5
-Log(LC50)DM	Log(mol/L)	2.53	N/A	0.91	0.59
-Log(LD50)	Log(mol/kg)	1.26	N/A	1.76	0.81
Log(BCF)	-	-0.41	N/A	0.38	0.73
-Log(PEL)	Log(mol/m3)	3.38	N/A	3.71	1.38
-Log(PCO)	-	0.73	N/A	1.13	0.39
Log(GWP)	-	N/A	N/A	N/A	N/A
Log(ODP)	-	N/A	N/A	N/A	N/A
Log(AP)	-	N/A	N/A	N/A	N/A
-LOG(EUAC)	Log(cas/kg)	5.97	N/A	5.26	5.73
-LOG(EUANonC)	Log(cas/kg)	6.41	N/A	7.96	6.61
-LOG(ERAC)	Log(cas/kg)	7.04	N/A	5.89	6.97
-LOG(ERANonC)	Log(cas/kg)	6.93	N/A	8.6	7.55
-LOG(EFWC)	Log(cas/kg)	6.38	N/A	5.64	6.24
-LOG(EFWNonC)	Log(cas/kg)	6.66	N/A	8.76	6.69
-LOG(ESWC)	Log(cas/kg)	9.35	N/A	7.91	9.02
-LOG(ESWNonC)	Log(cas/kg)	9.87	N/A	10.93	8.79
-LOG(ENSC)	Log(cas/kg)	6.85	N/A	6.2	6.92
-LOG(ENSNonC)	Log(cas/kg)	6.57	N/A	8.88	6.78
-LOG(EASC)	Log(cas/kg)	6.6	N/A	5.76	6.67
-LOG(EASNonC)	Log(cas/kg)	6.35	N/A	8.54	6.8
Secondary properties					
Zc	-	0.211	N/A	0.23	0.24
Sfus	J/(mol*K)	40.48	N/A	52.46	31
Vm[Tb]	cm^3/mol	65.71	N/A	108.5	60.85
Refractive Index	-	1.372	1.3632	1.3901	1.3611
Molar Refraction	-	19.3	N/A	37.88	26.08
Closed Flash Temp.	K	N/A	N/A	325.63	281.4
Open Flash Temp.	K	327.32	N/A	319.26	286.42
Dipolar moment	debye	1.44	N/A	2.49	1.72
Dielectric const.	-	7.15	N/A	15.45	23.07
Henry[298K]	$bar*m^3/mol$	1.01E-07	2.33E-01	0.00	5.07E-06

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Physical properties

Chemical	Unit	Acetic acid	Ethylene	Acetic anhydride	Ethyl alcohol
CAS no.		64-19-7	74-85-1	108-24-7	64-17-5
McGowan Volume	cm^3/mol	46.48	N/A	76.23	44.91

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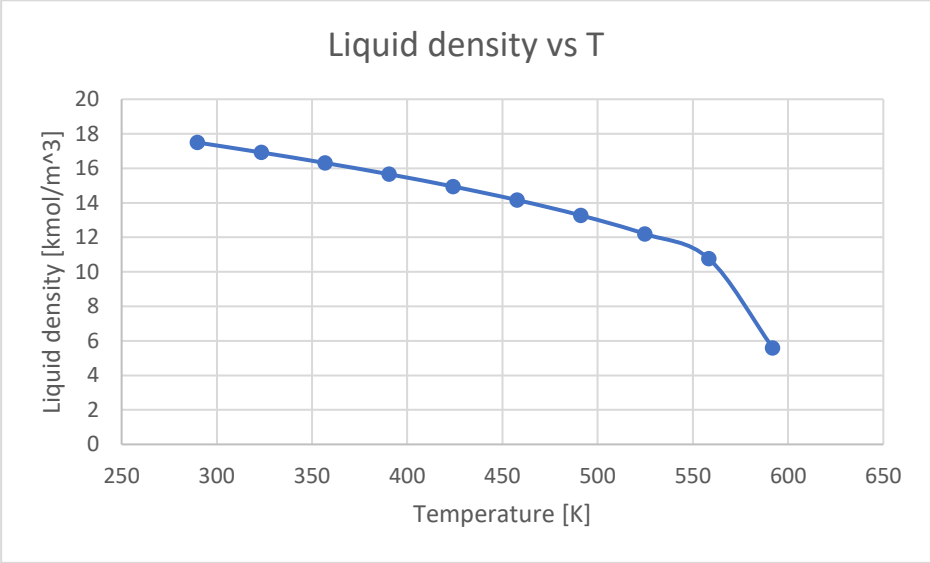
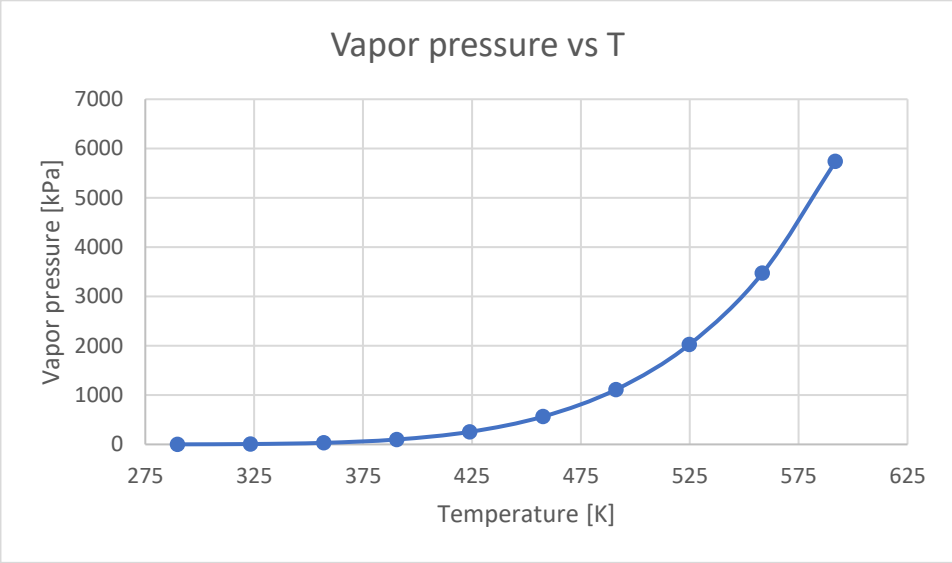
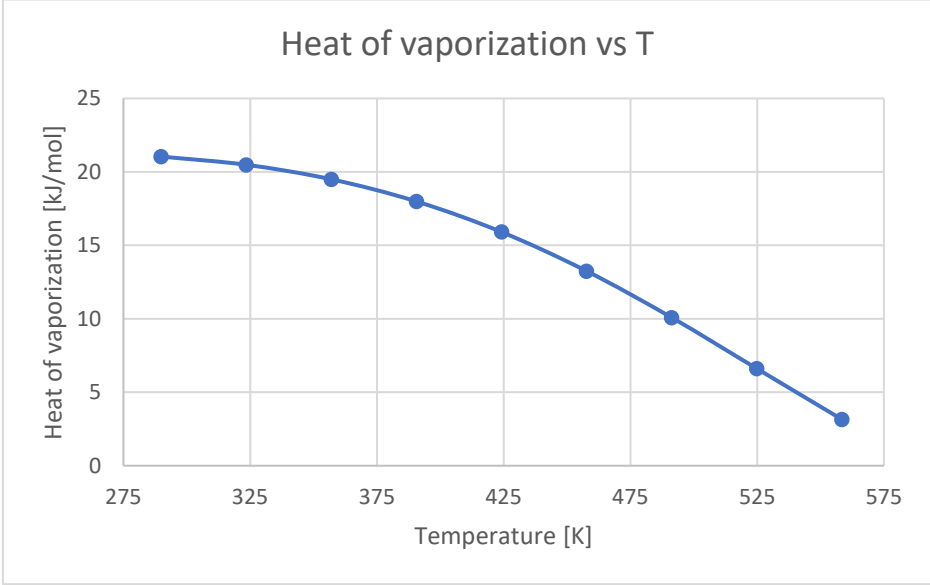
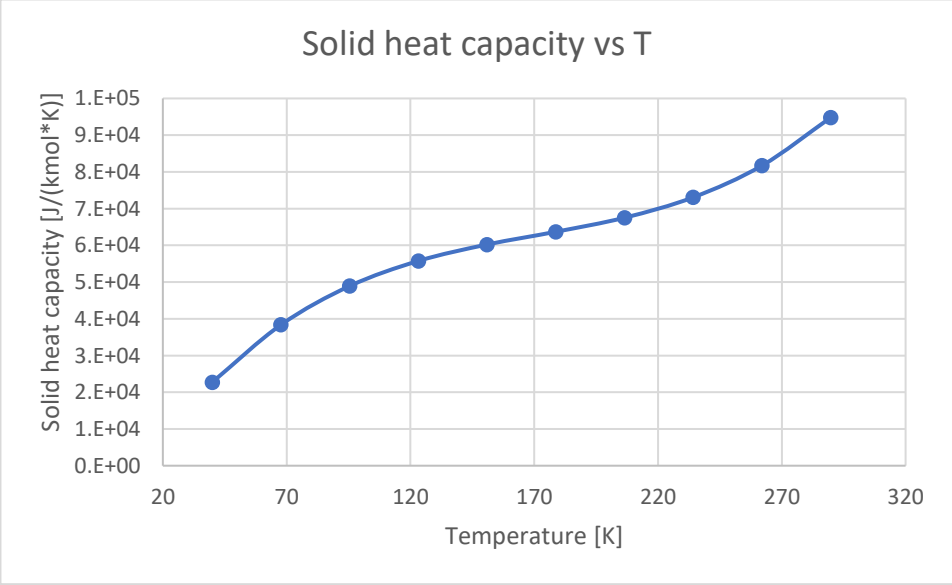
Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

Chemical Acetic acid









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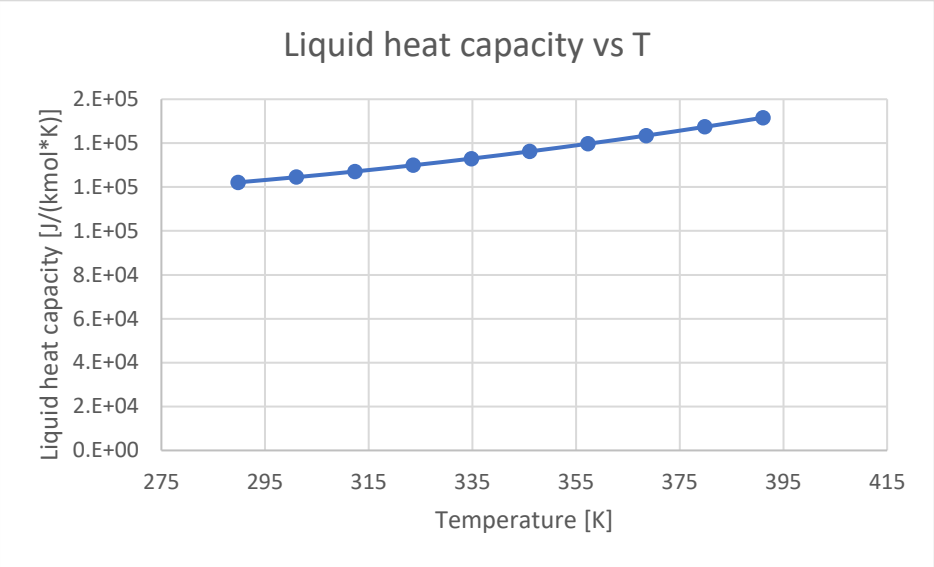

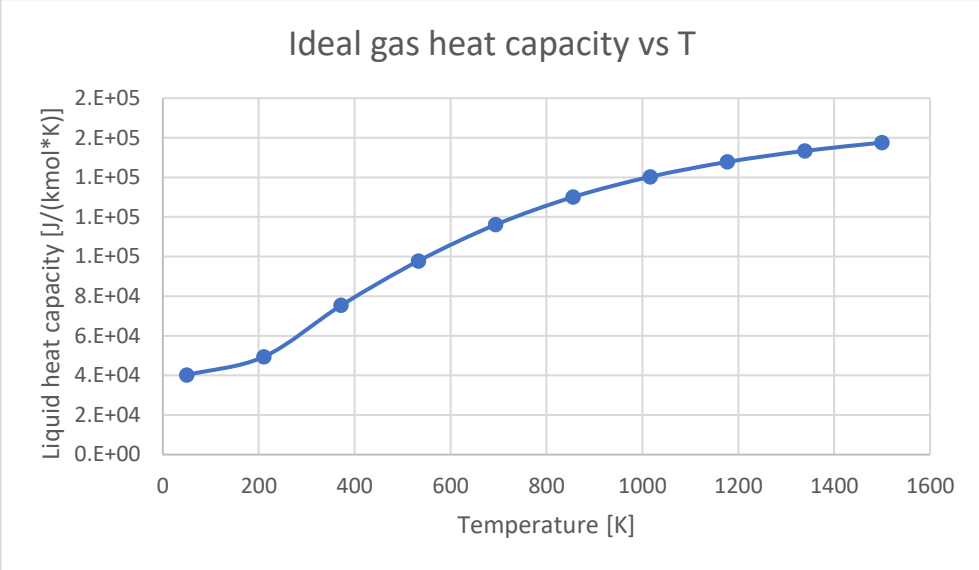

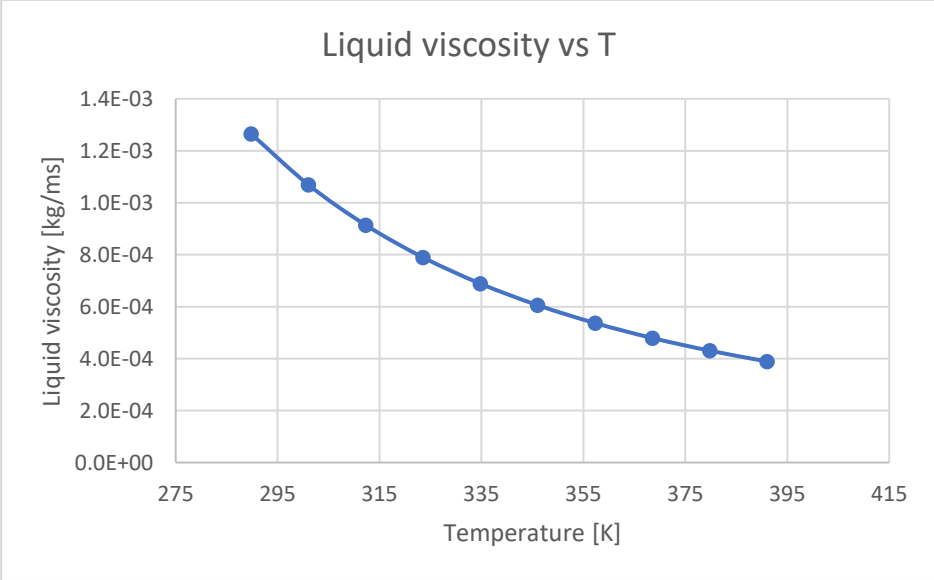

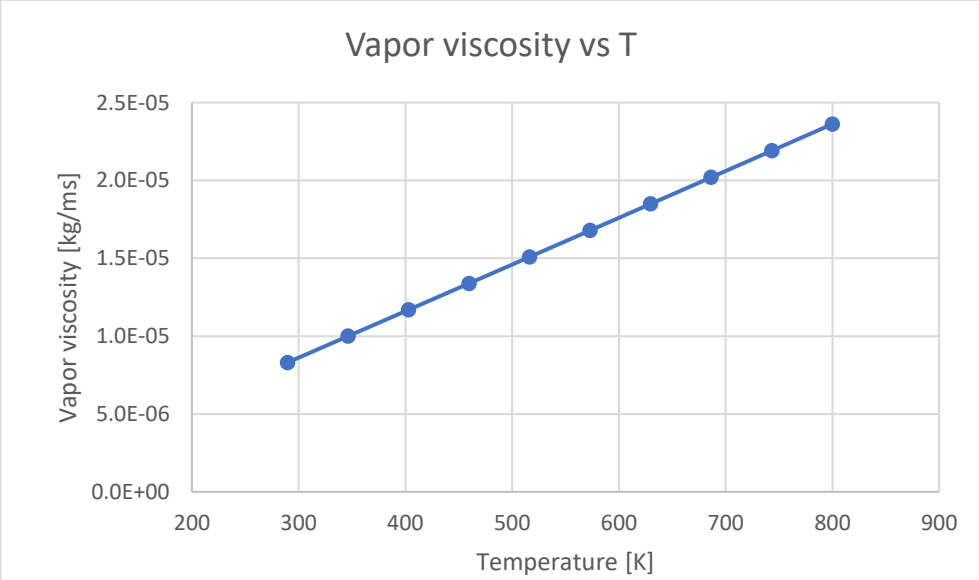

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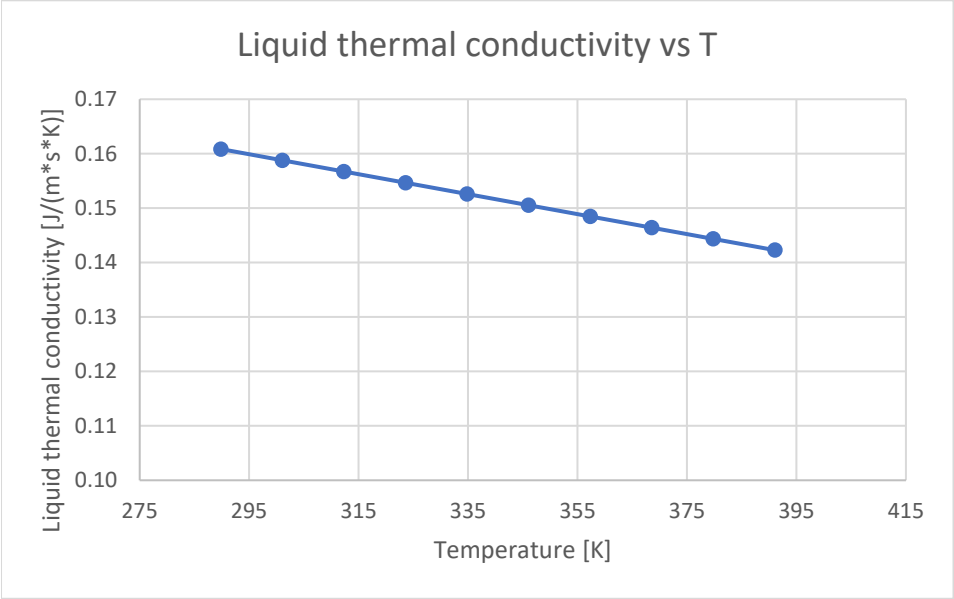

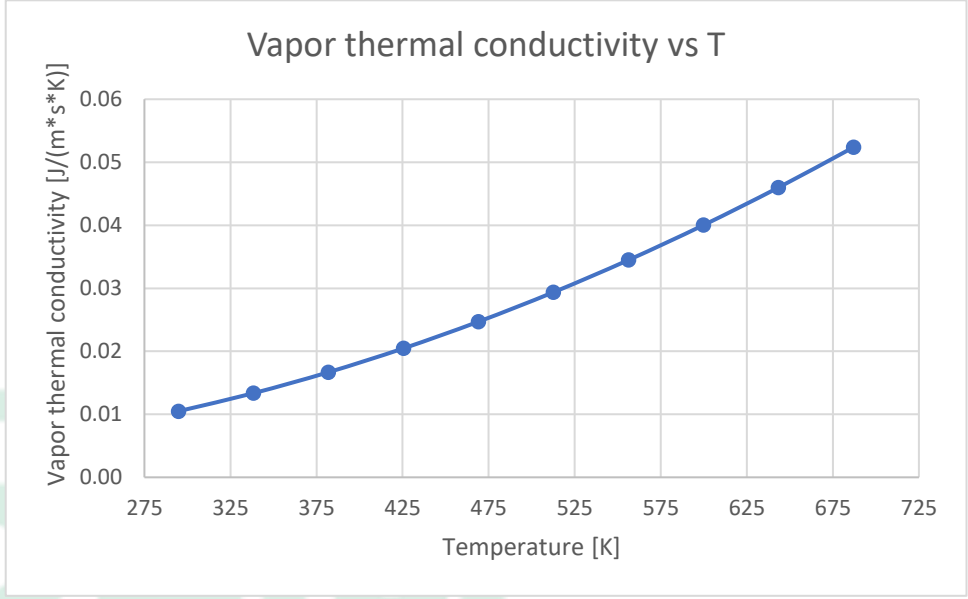

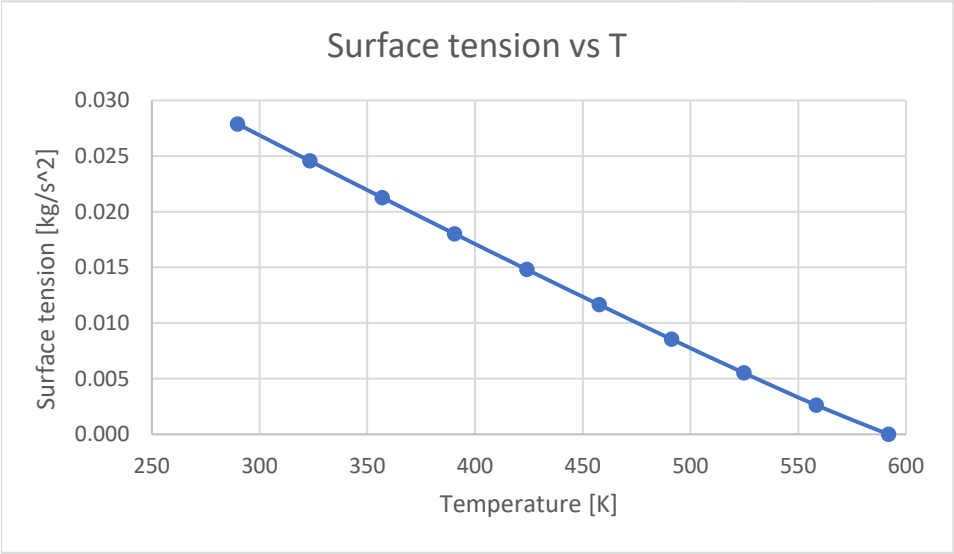

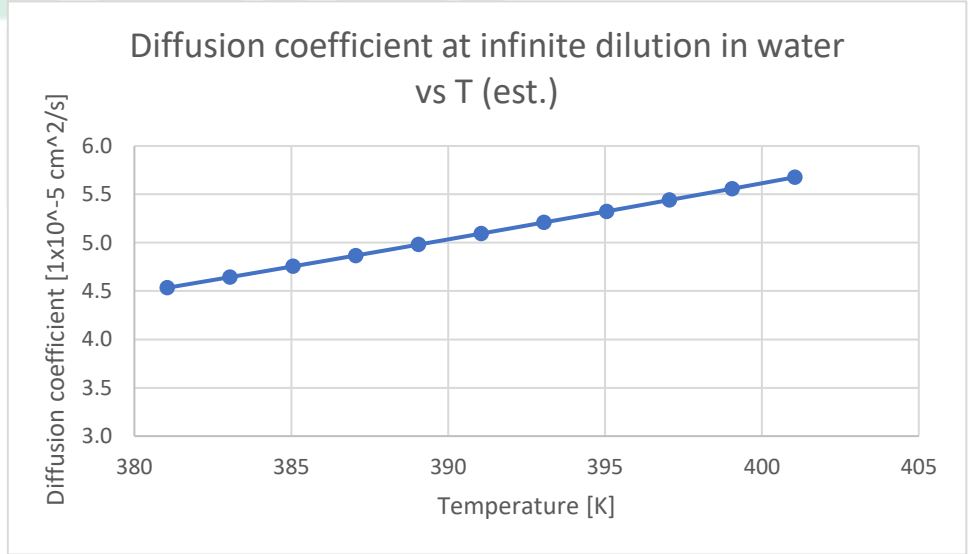

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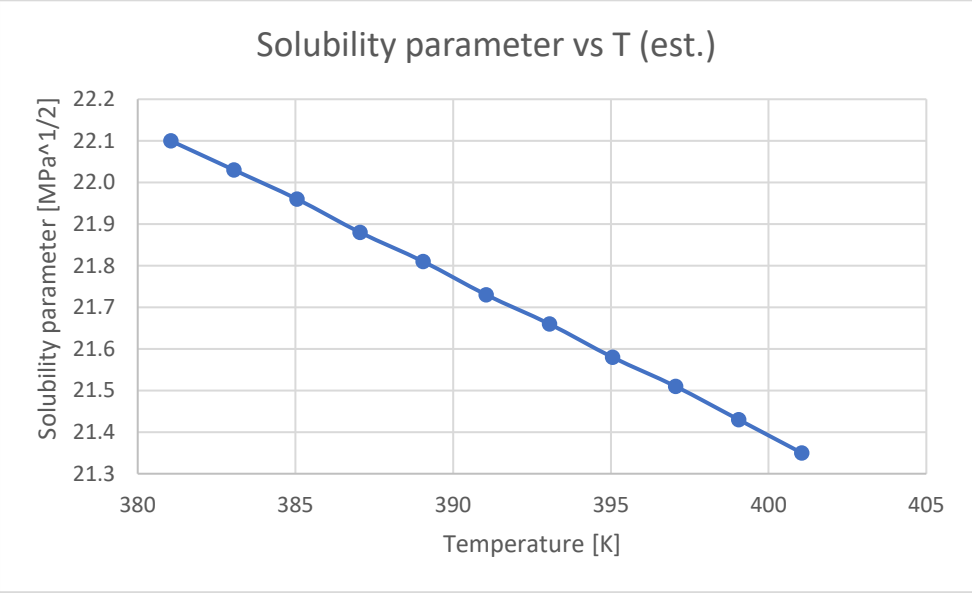

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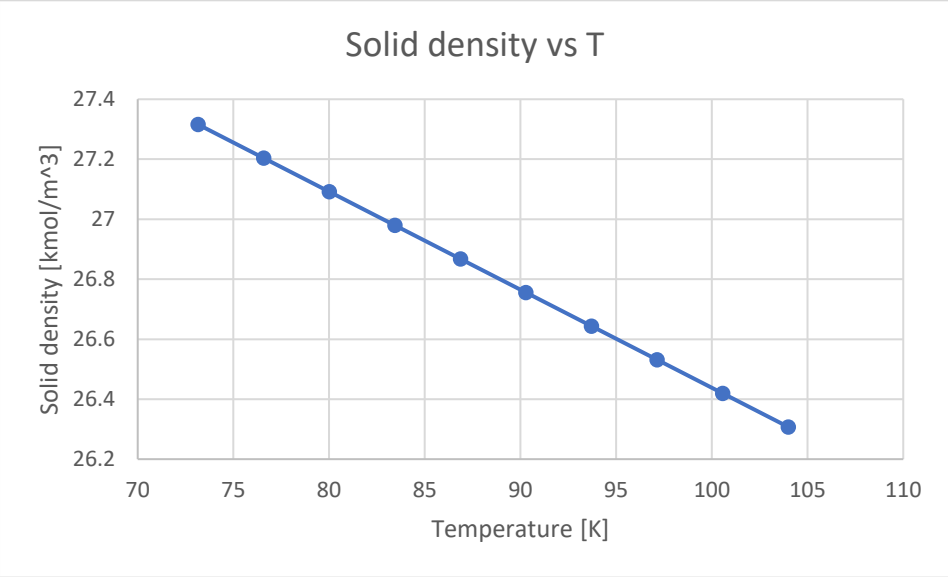
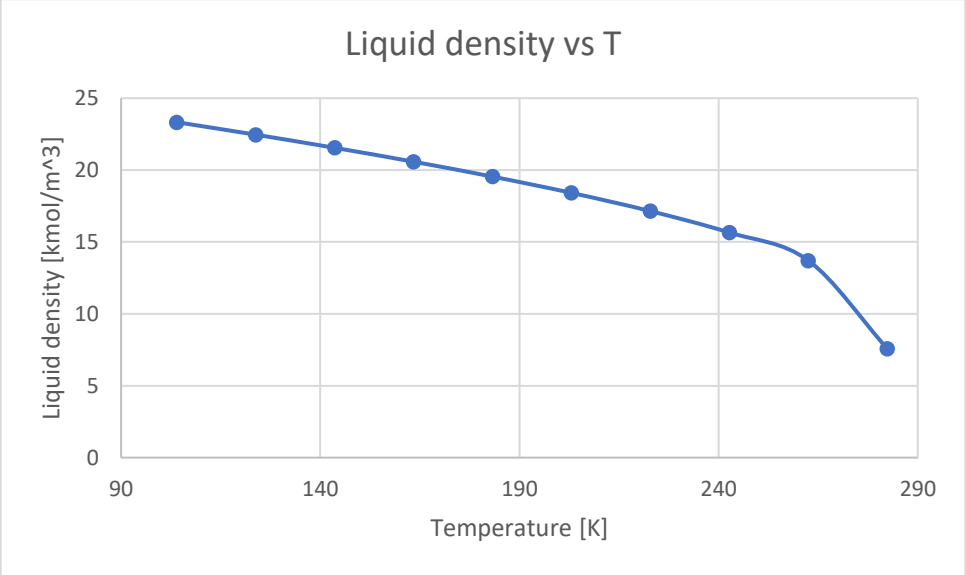
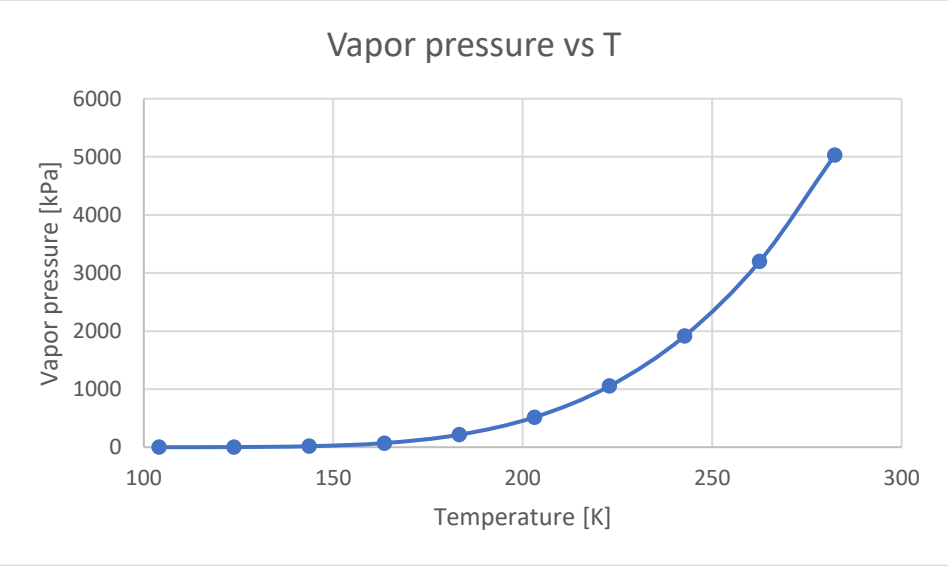
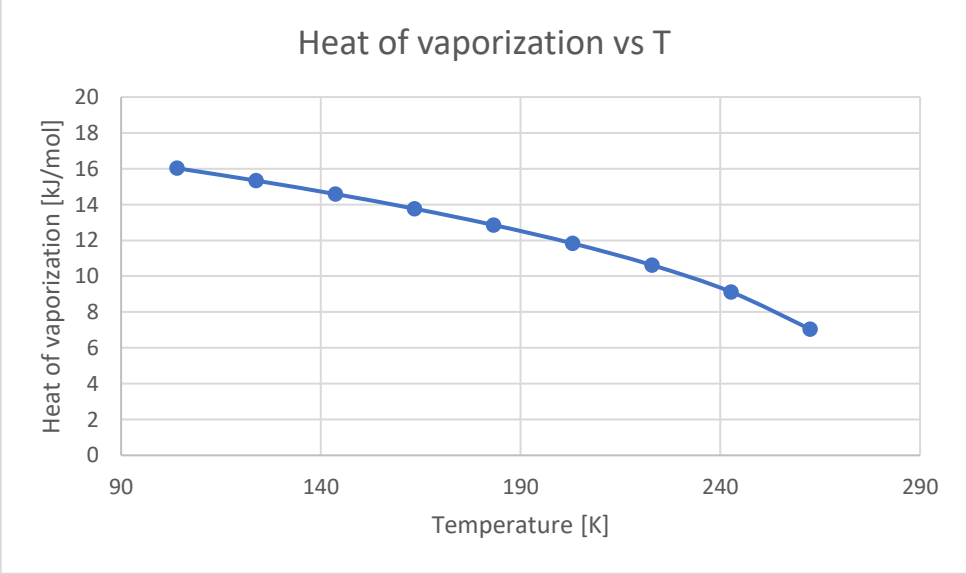
Chemical Ethylene









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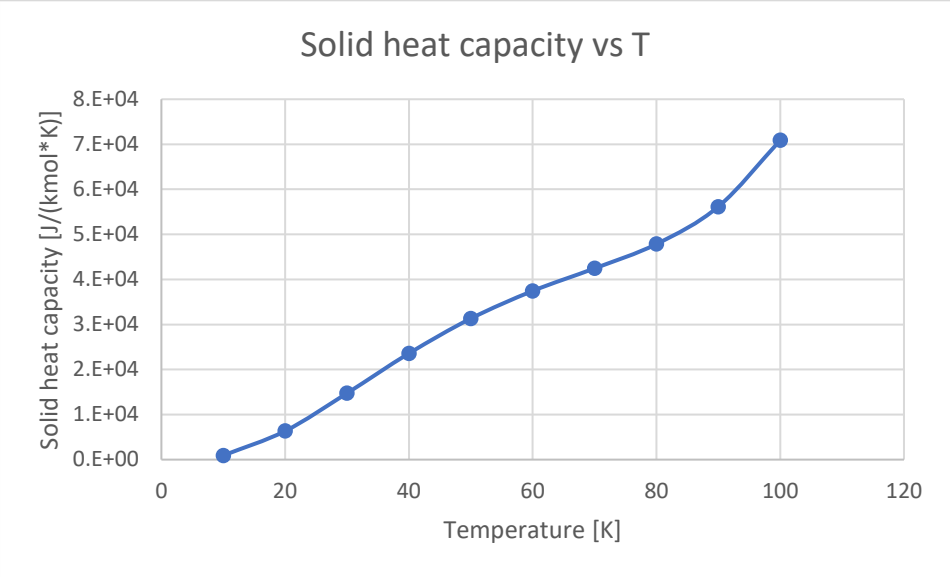

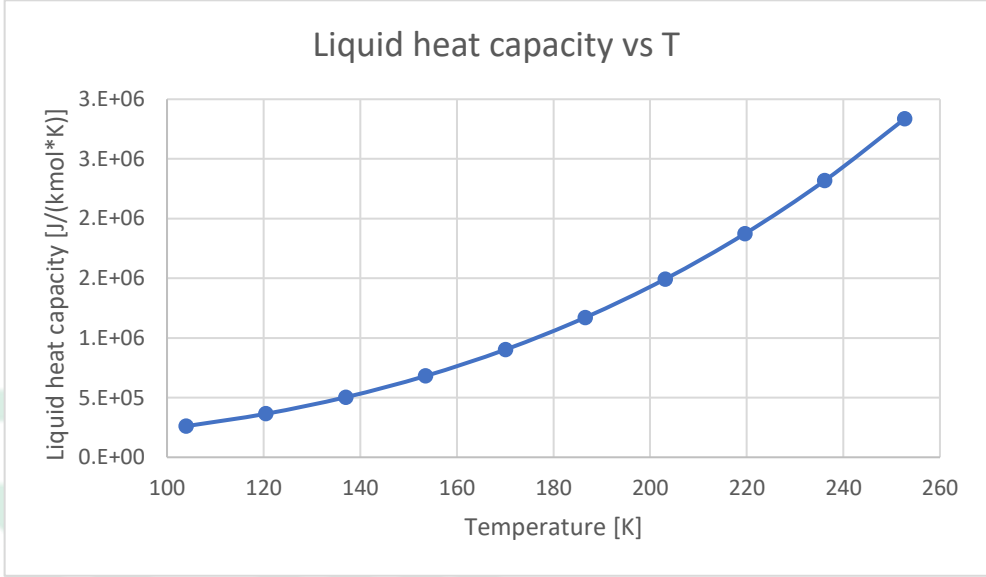

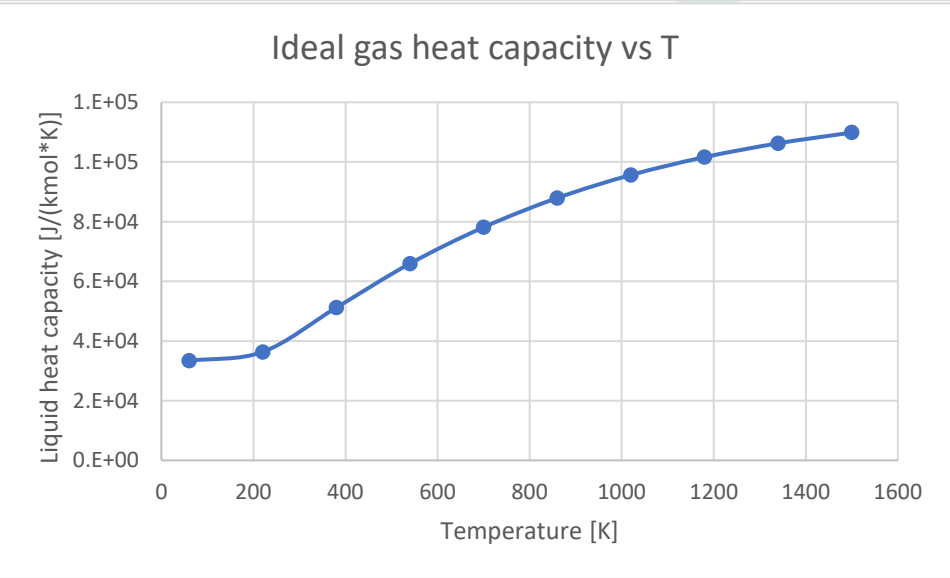

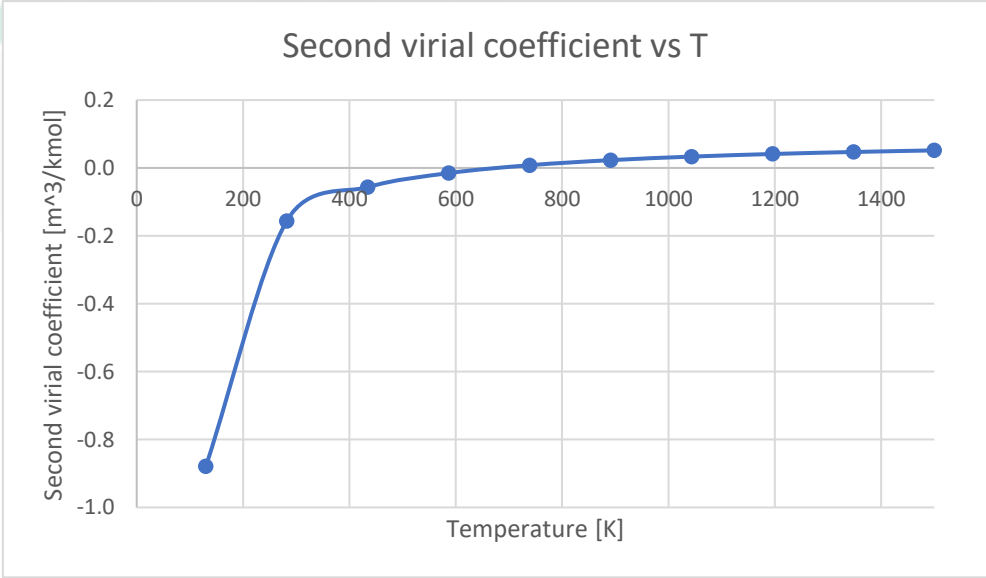

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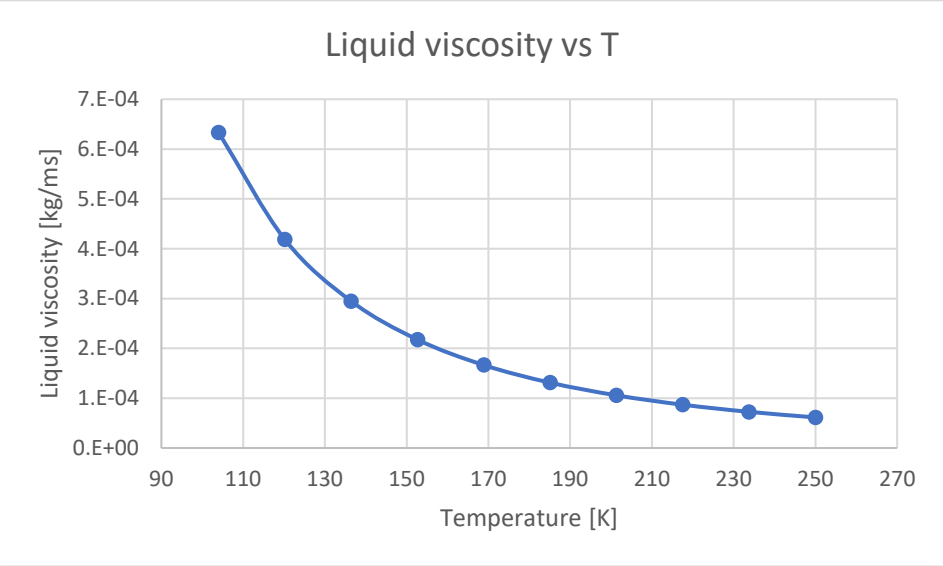

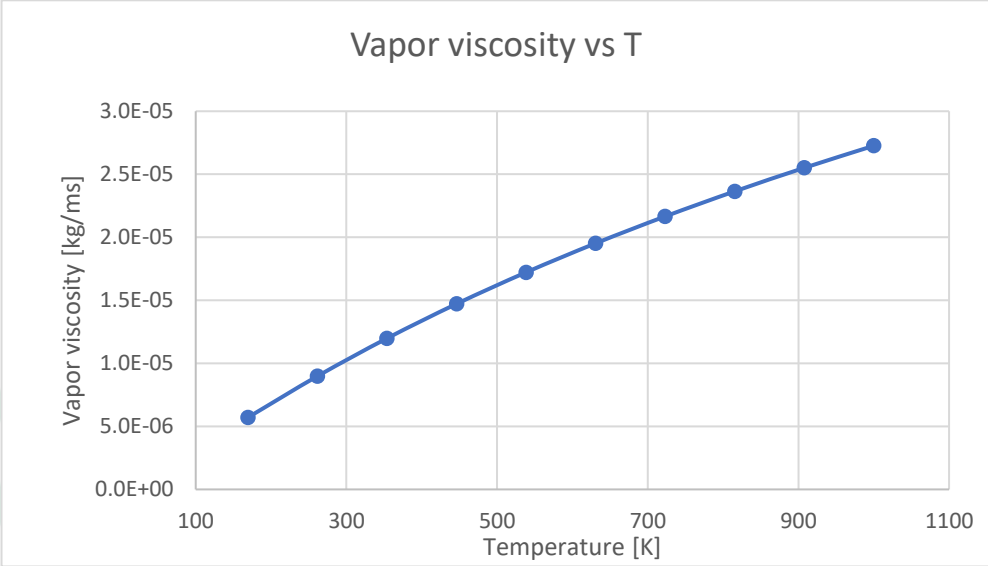

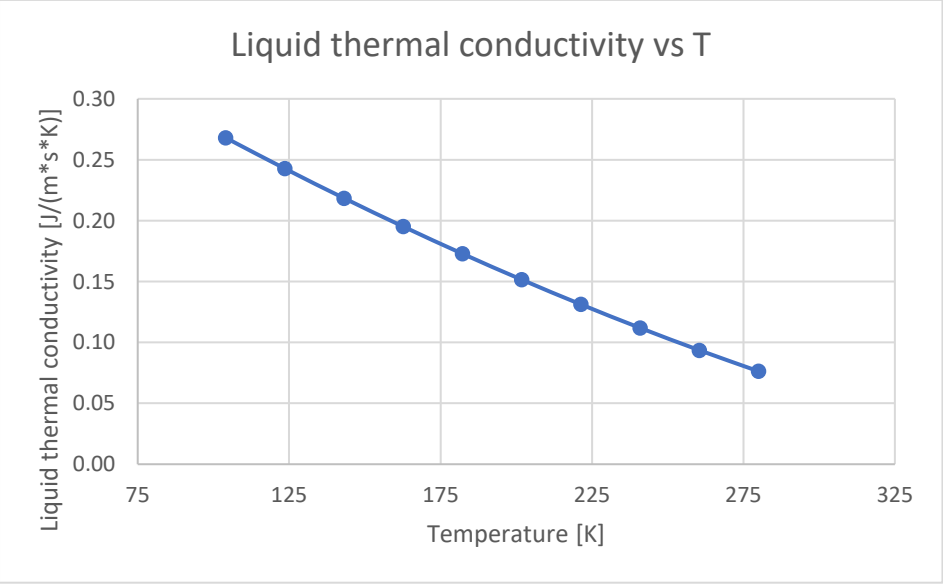

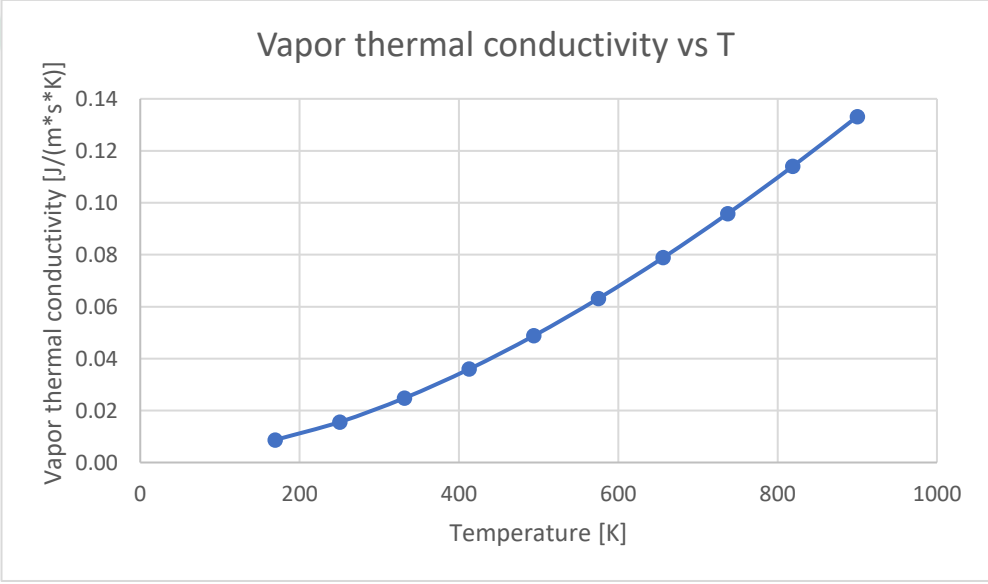

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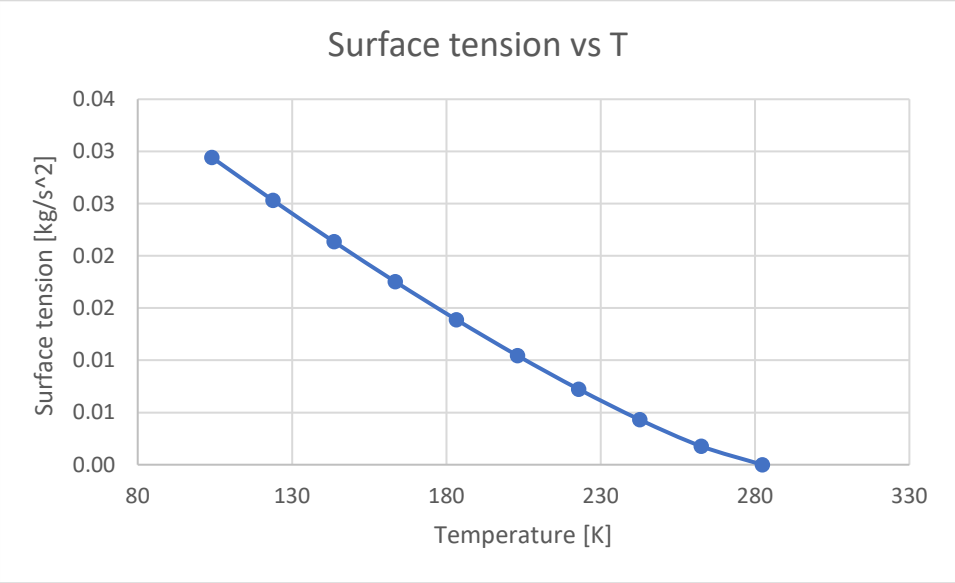

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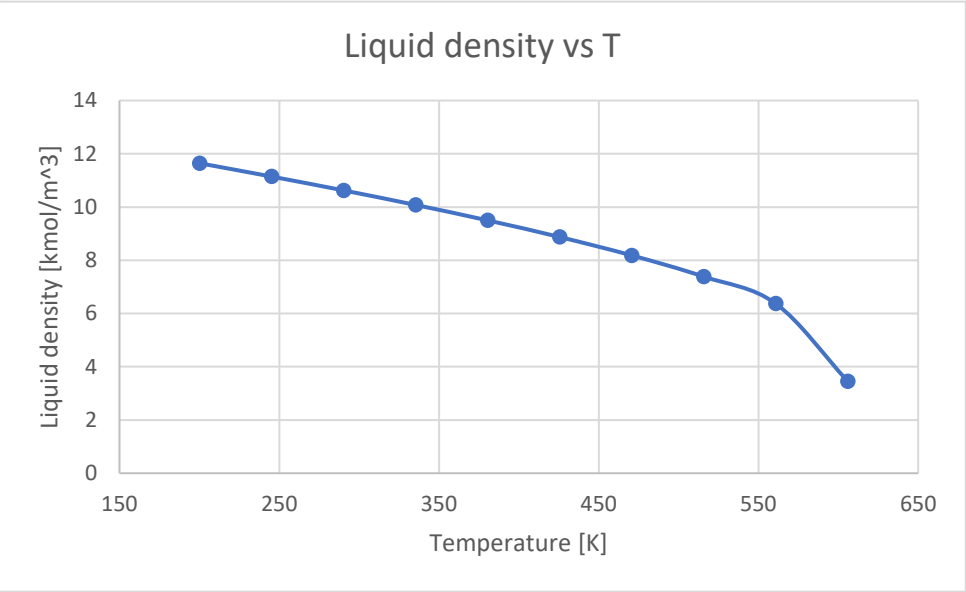
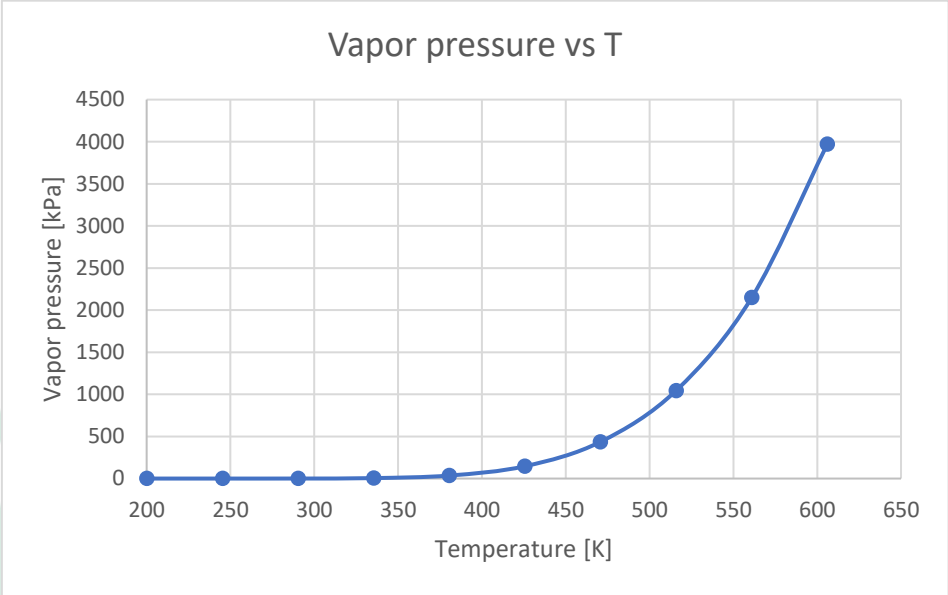
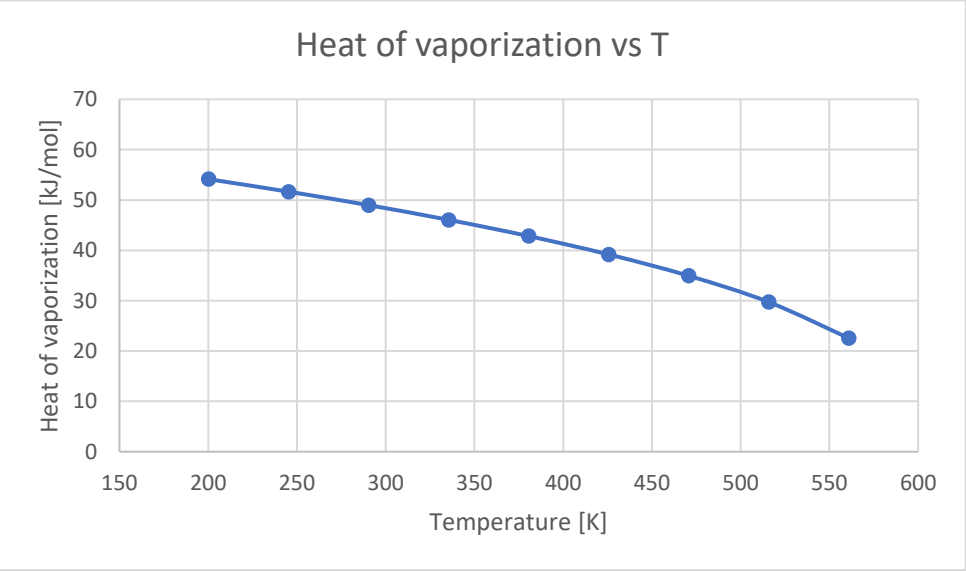
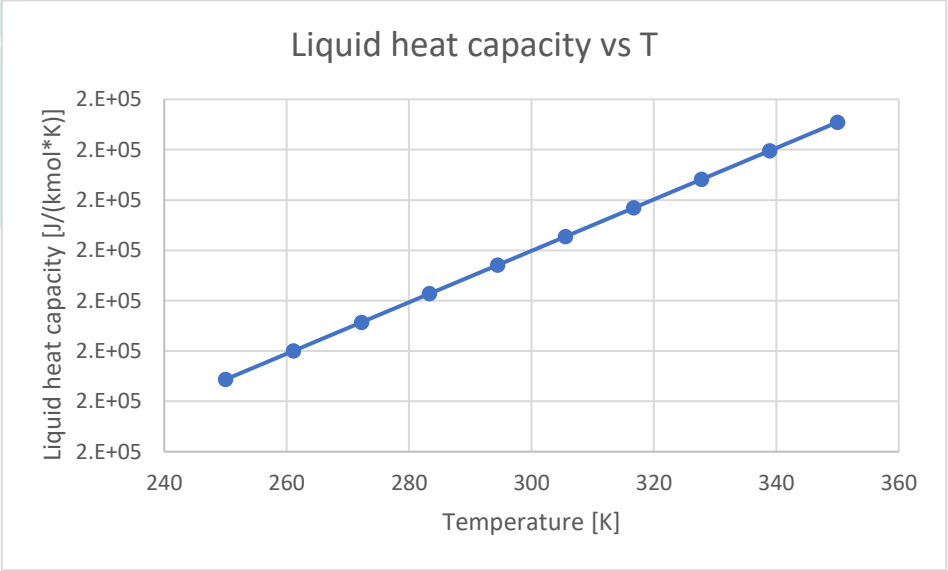
Chemical Acetic anhydride









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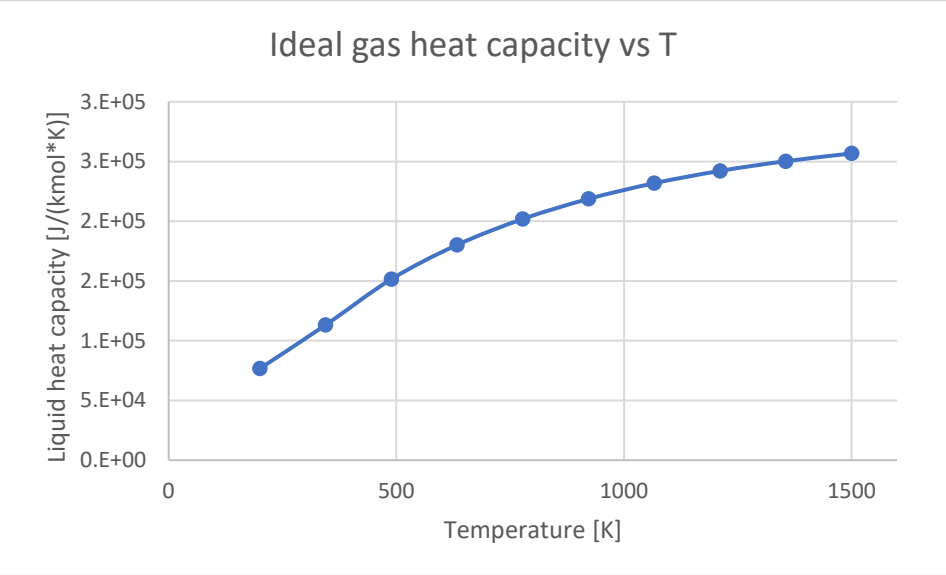

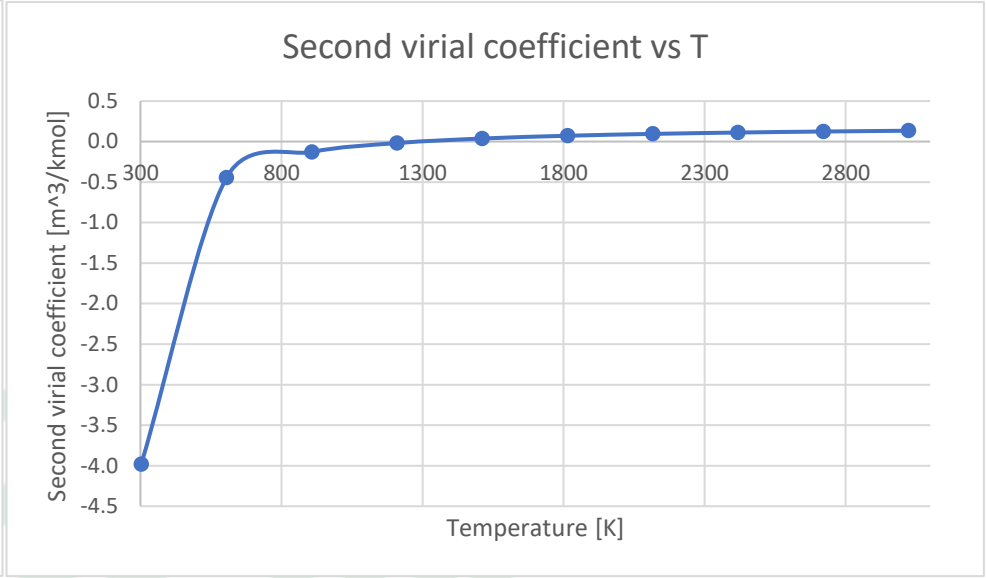

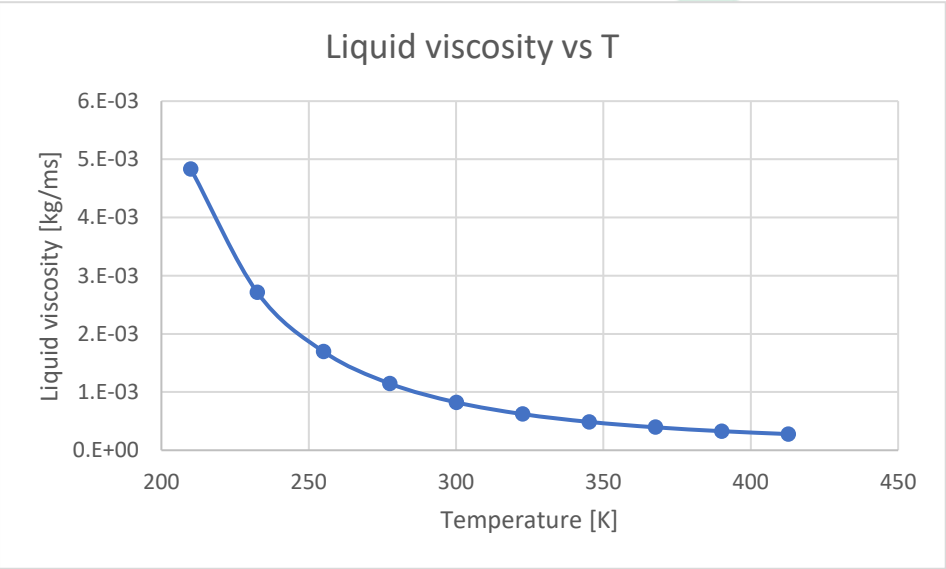

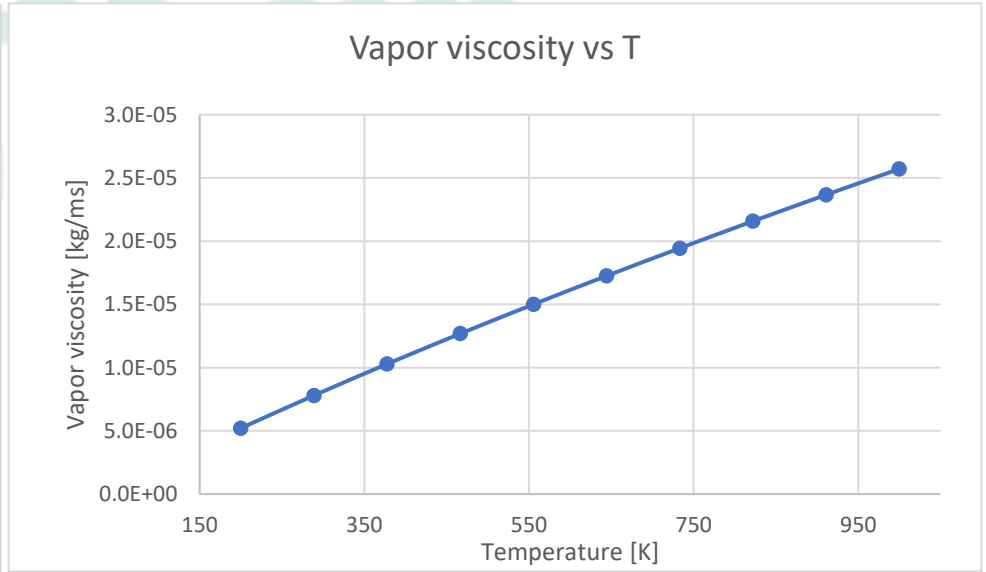

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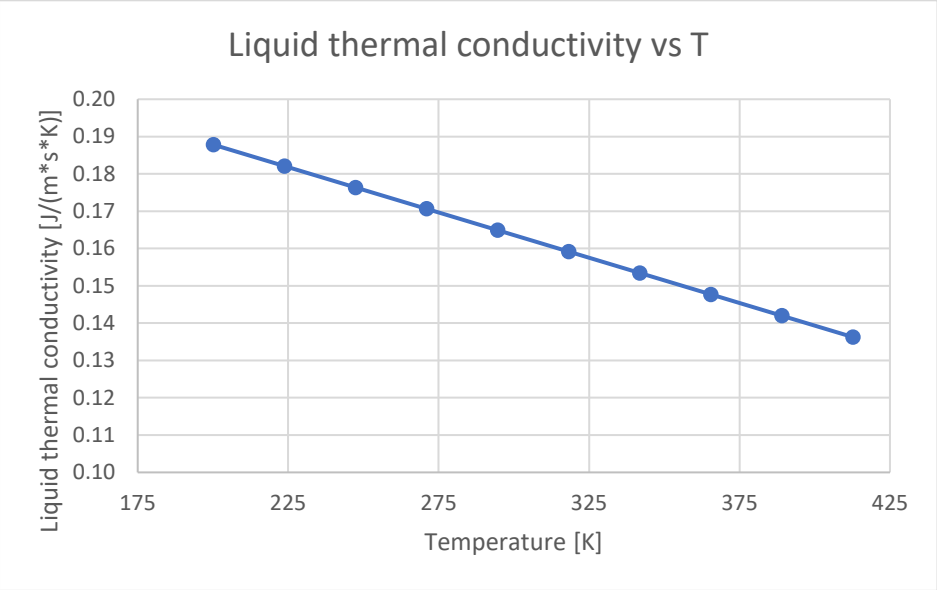

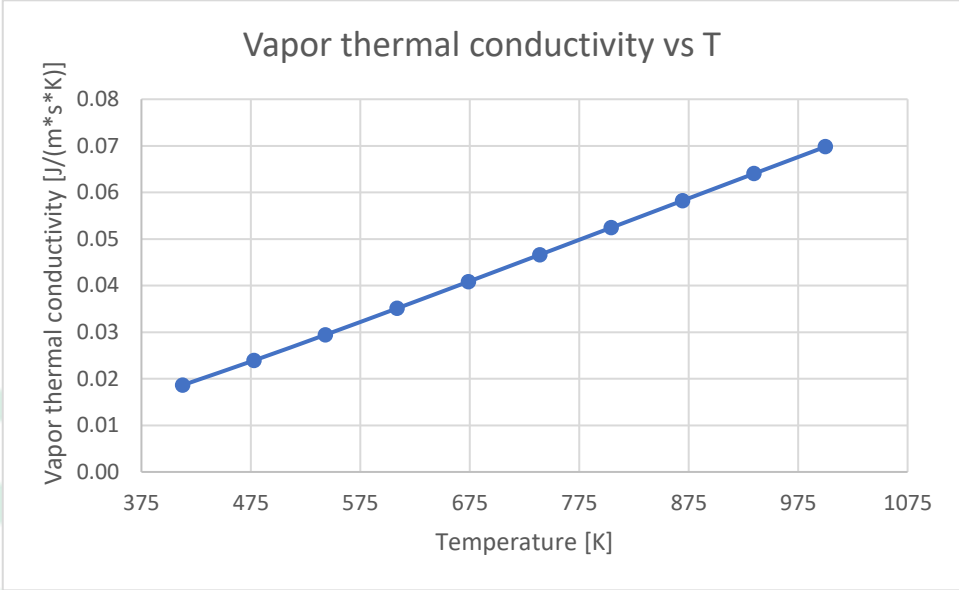

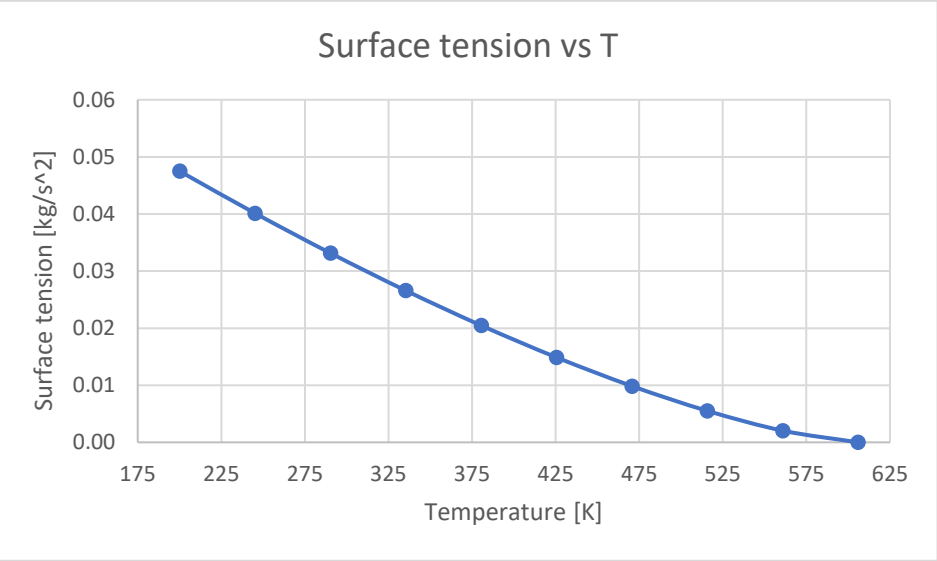

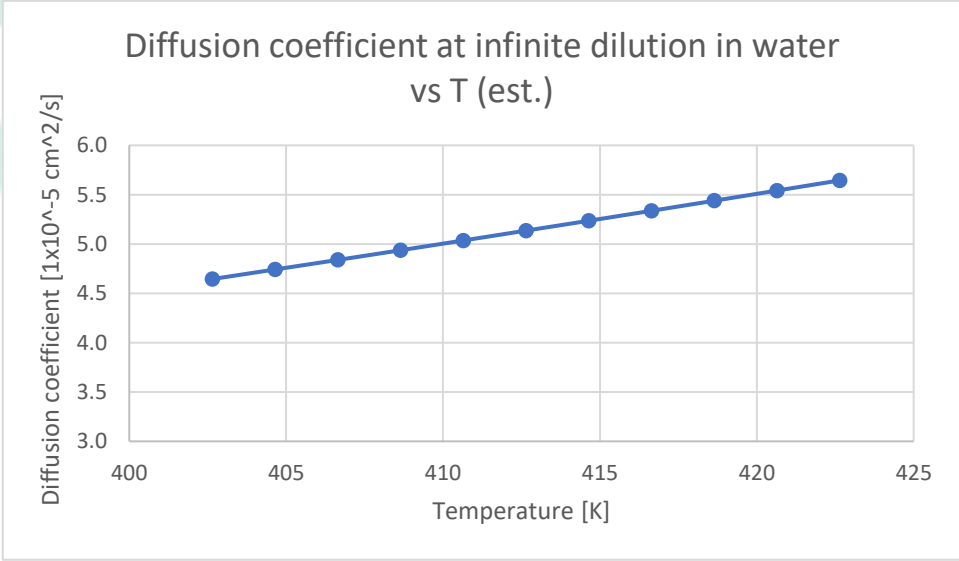

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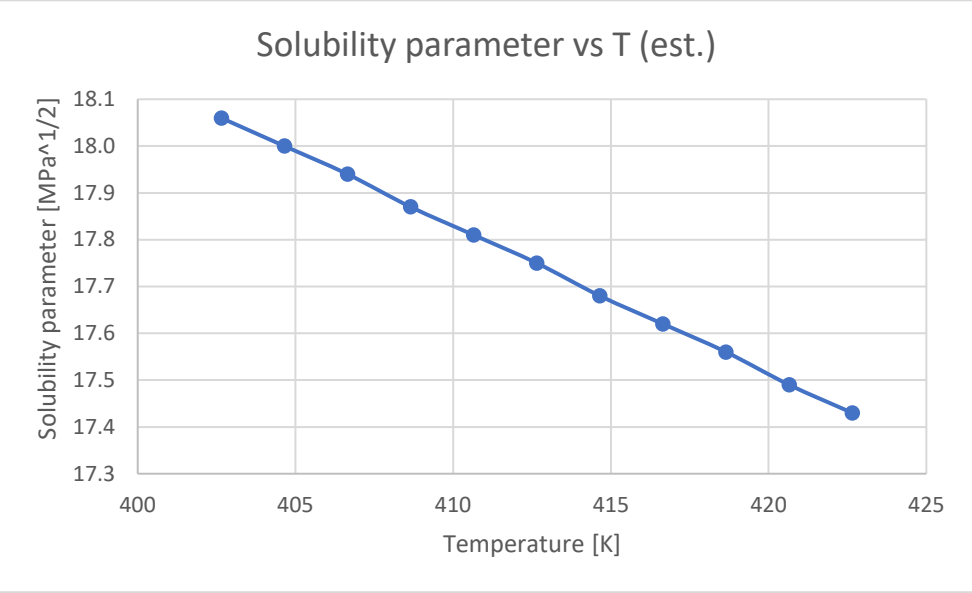

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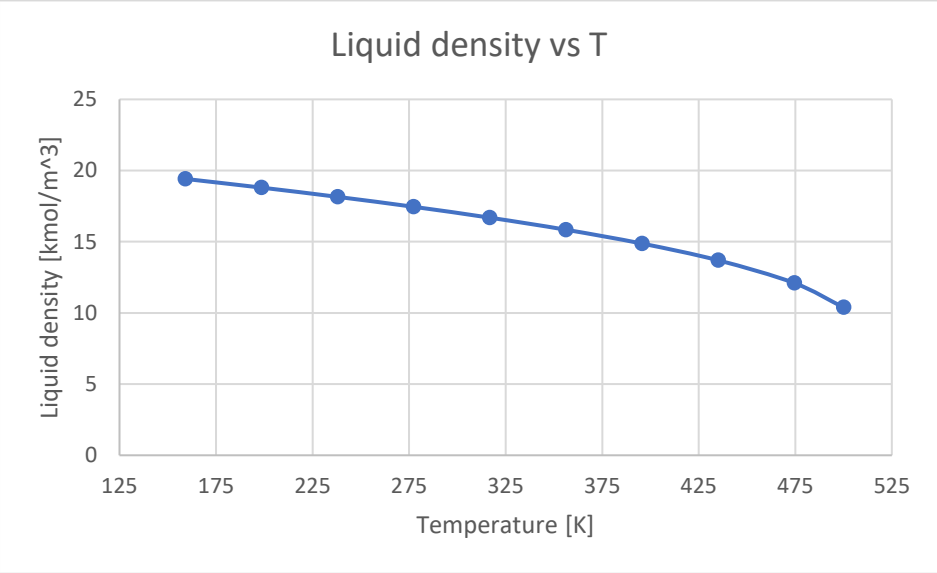

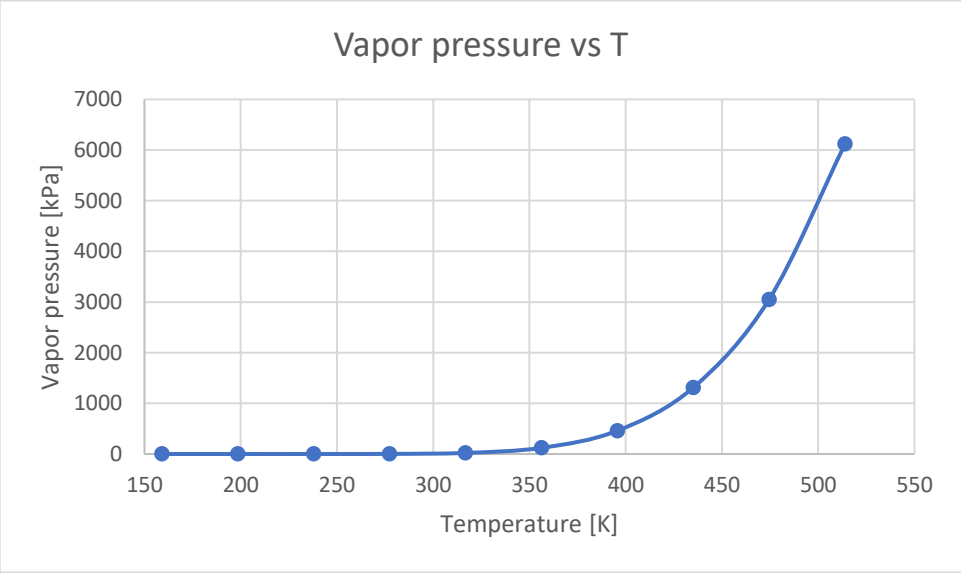

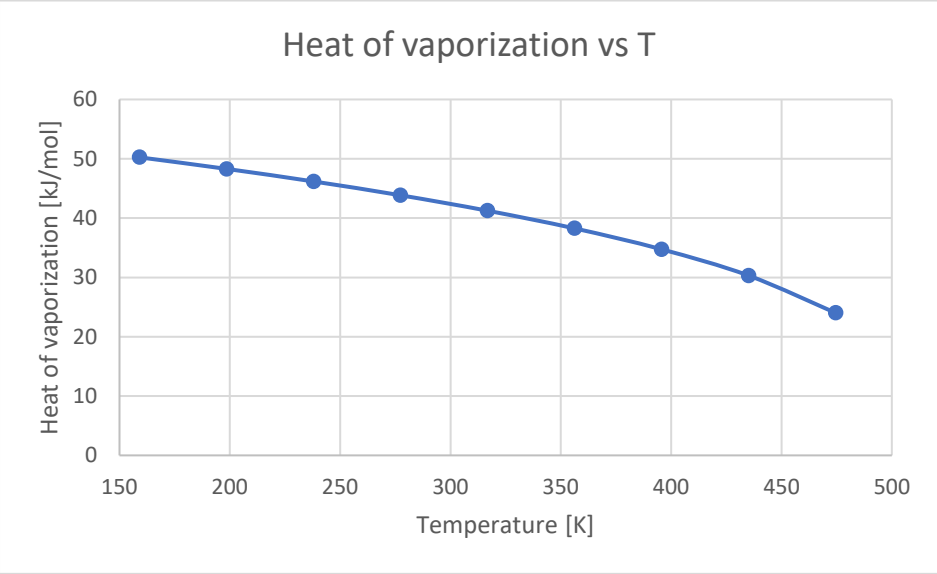

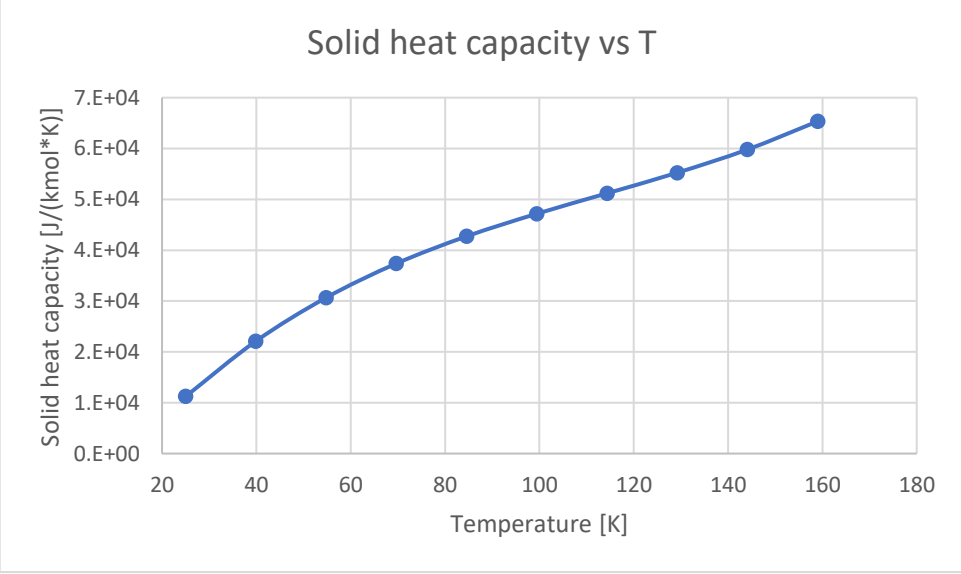

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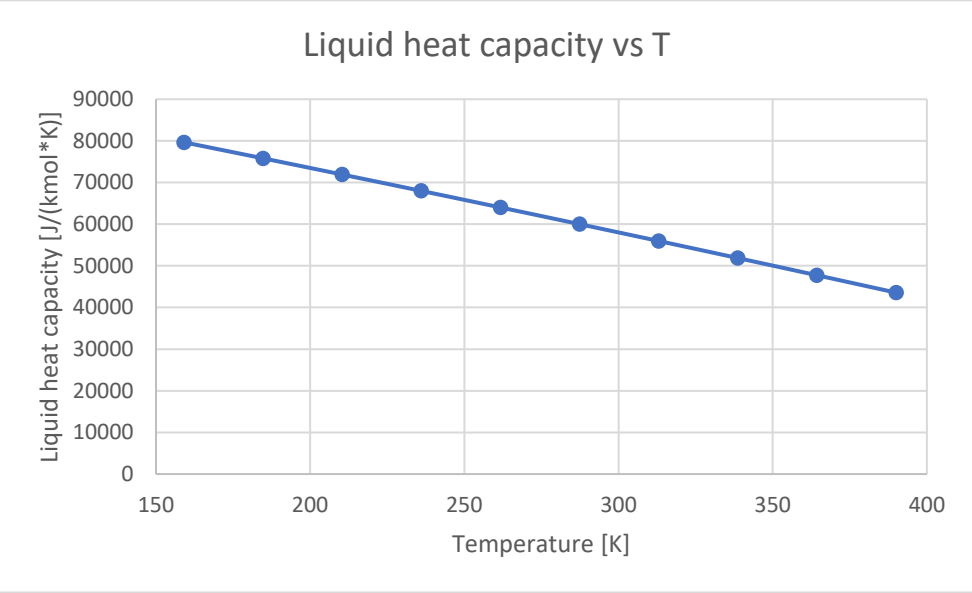
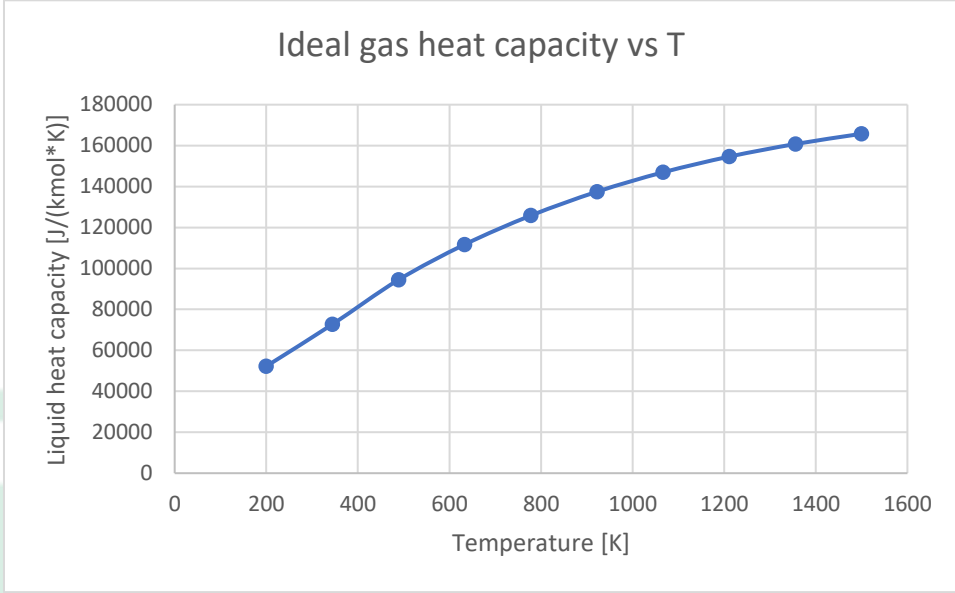
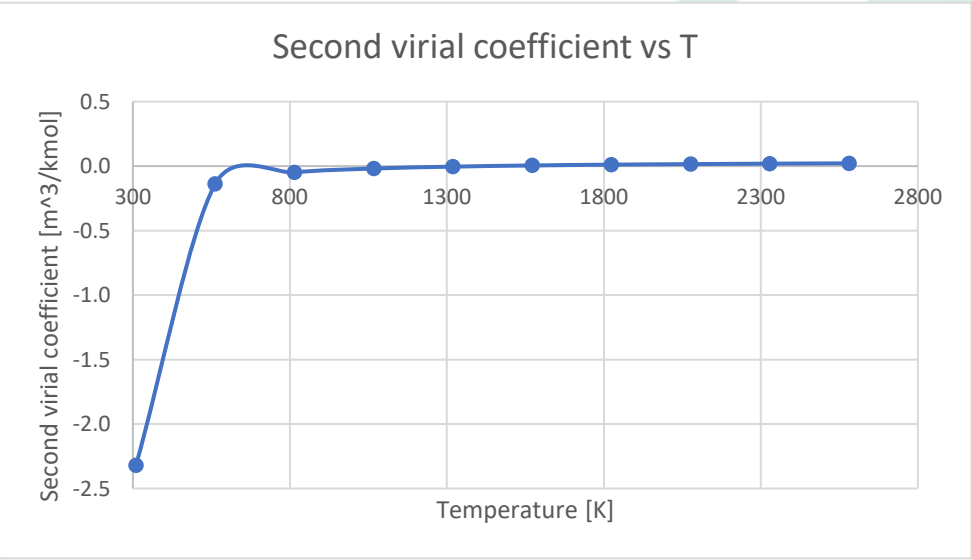
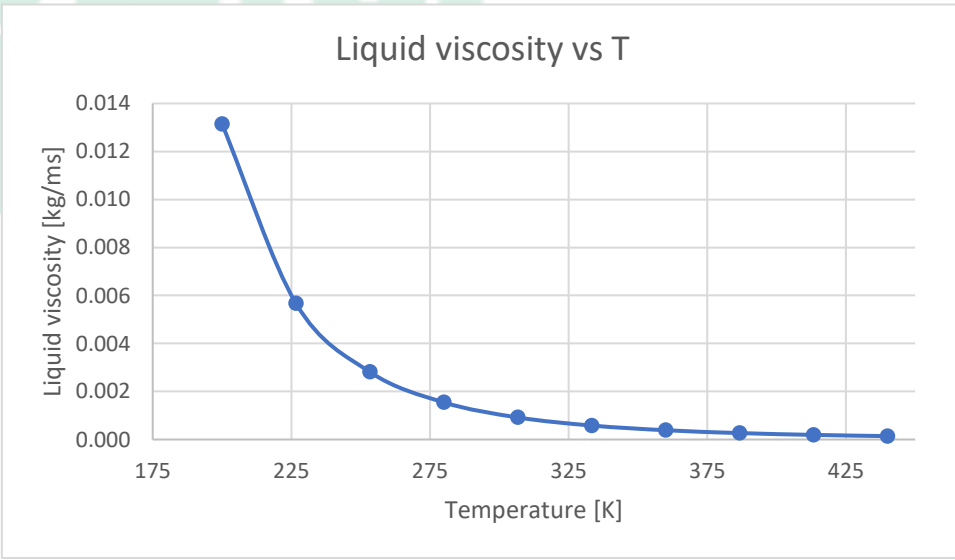
Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

Chemical Ethyl alcohol









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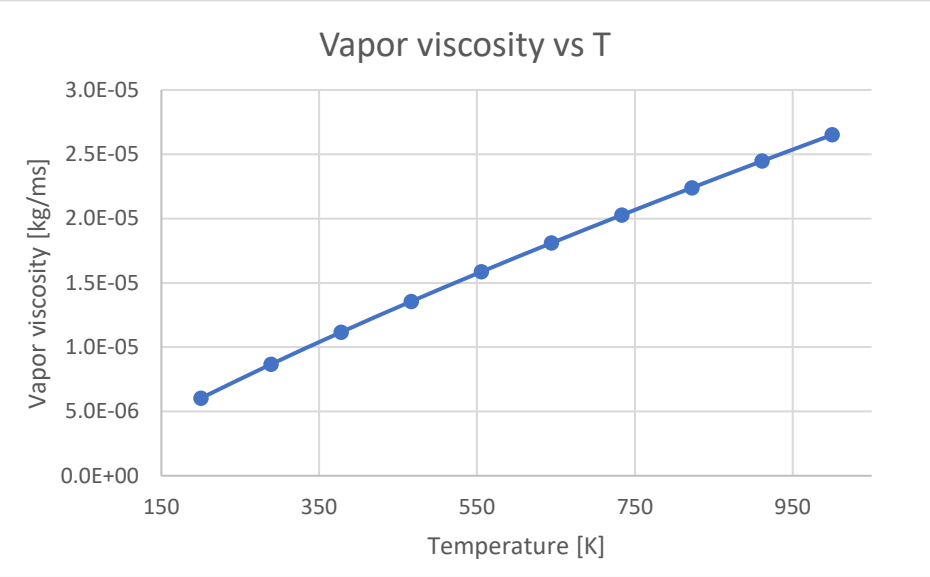

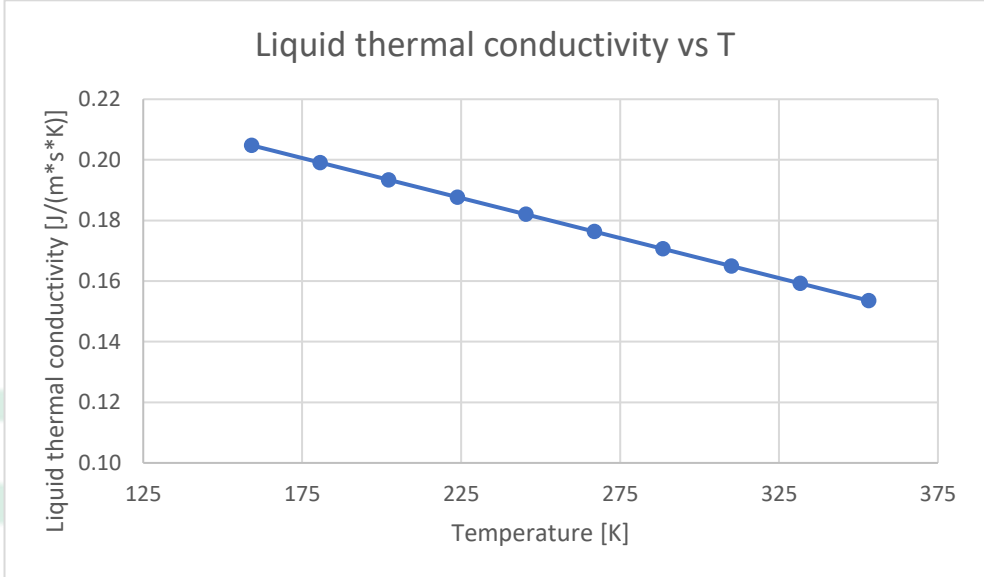

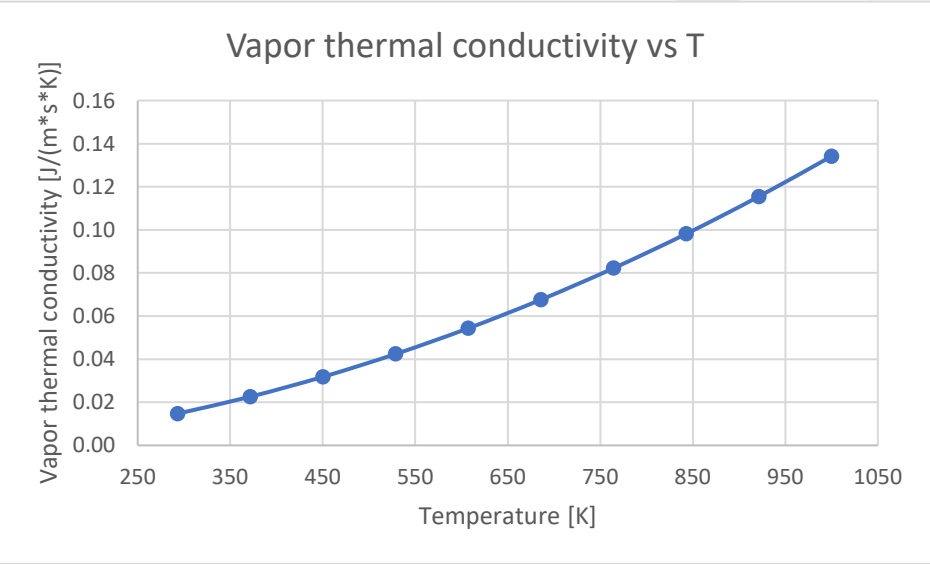

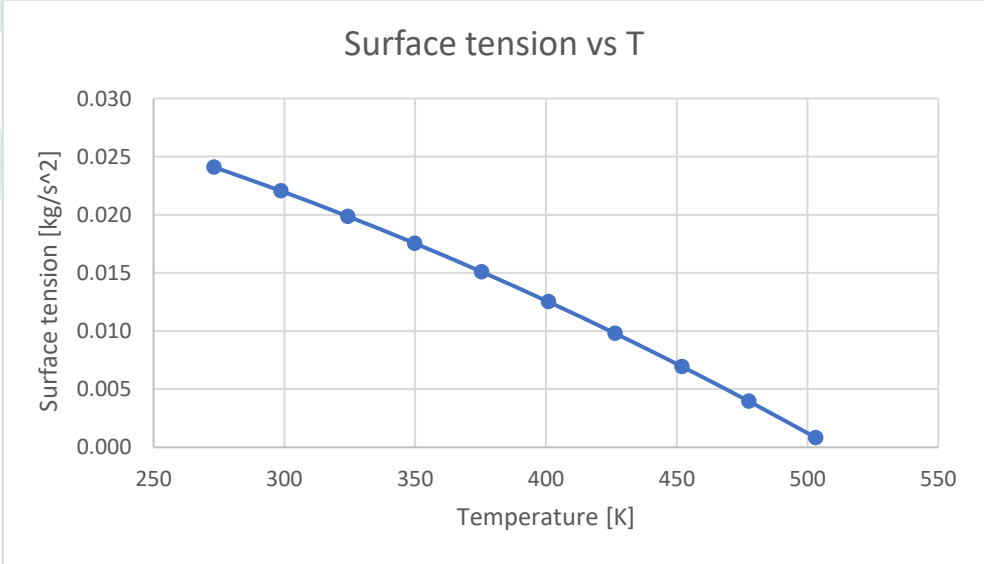

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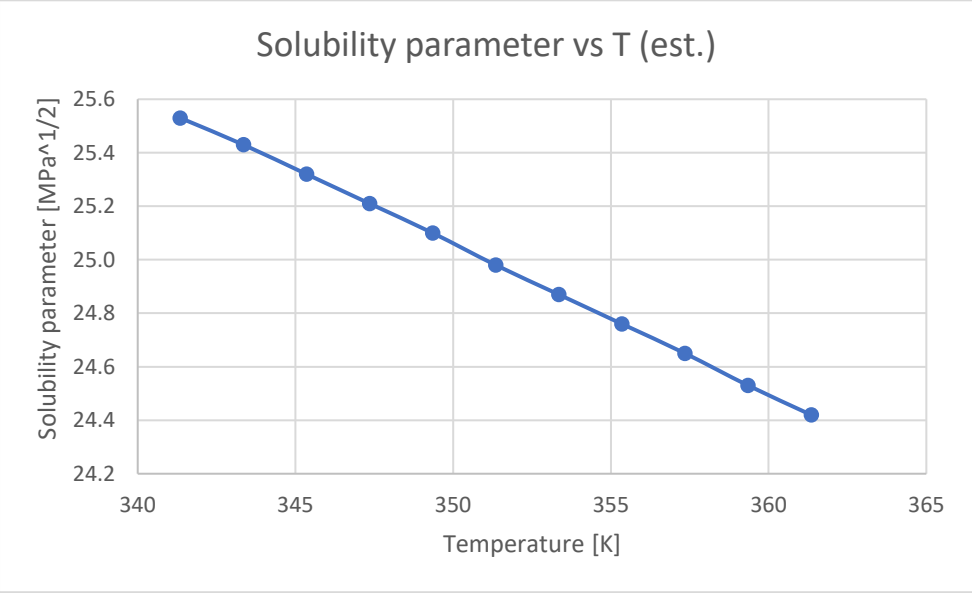

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Chemical	Acetic acid	Ethylene	Acetic anhydride	Ethyl alcohol
CAS no.	**64-19-7**	**74-85-1**	**108-24-7**	**64-17-5**
Physical hazard				
Flammable gases		D(H220)		
Flammable liquids	W(H226)		W(H226)	D(H225)
Gases under pressure		W(H280, H281)		
Corrosive to Metals			W(H290)	
Health hazard				
Acute toxicity, oral	W(H303)		W(H302)	
Acute toxicity, dermal	W(H312)		H313	
Skin corrosion/irritation	D(H314)		D(H314)	
Sensitization, Skin				
Serious eye damage/eye irritation	D(H318)		D(H318)	W(H319, H320)
Acute toxicity, inhalation		W(H336)	D(H330, H331) W(H332)	
Sensitization, respiratory	D(H334)			
Specific target organ toxicity, single exposure; Respiratory tract irritation			W(H336)	W(H335, H336)
Germ cell mutagenicity				D(H340)
Carcinogenicity				D(H350)
Reproductive toxicity				D(H360)
Specific target organ toxicity, single exposure	D(H370) W(H371)		D(H370)	W(H371)
Specific target organ toxicity, repeated exposure		W(H373)	D(H372)	D(H372) W(H373)
Environmental hazard				
Hazardous to the aquatic environment, acute hazard		H402		
Hazardous to the aquatic environment, long-term hazard		H412		H412

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Physical hazard statement

Code	Hazard Class (GHS Chapter)	Hazard Category	Signal Word
	Explosives		
H200	Unstable Explosive	Unstable Explosive	Danger
H201	Explosive; mass explosion hazard	Div 1.1	Danger
H202	Explosive; severe projection hazard	Div 1.2	Danger
H203	Explosive; fire, blast or projection hazard	Div 1.3	Danger
H204	Fire or projection hazard	Div 1.4	Warning
H205	May mass explode in fire	Div 1.5	Danger
	Desensitized explosives		
H206	Fire, blast or projection hazard; increased risk of explosion if desensitizing agent is reduced	Category 1	Danger
H207	Fire or projection hazard; increased risk of explosion if desensitizing agent is reduced	Category 2	Danger
H207	Fire or projection hazard; increased risk of explosion if desensitizing agent is reduced	Category 3	Warning
H208	Fire hazard; increased risk of explosion if desensitizing agent is reduced	Category 4	Warning
	Flammable gases		
H220	Extremely flammable gas	1A: Flammable gas, Pyrophoric gas, Chemically unstable gas A,B	Danger
H221	Flammable gas	1B	Danger
H221	Flammable gas	Category 2	Warning
	Flammable aerosol		
H222	Extremely flammable aerosol	Category 1	Danger
H223	Flammable aerosol	Category 2	Warning
	Flammable liquids		
H224	Extremely flammable liquid and vapor	Category 1	Danger
H225	Highly Flammable liquid and vapor	Category 2	Danger
H226	Flammable liquid and vapor	Category 3	Warning
H227	Combustible liquid	Category 4	Warning
	Flammable solids		
H228	Flammable solid	Category 1	Danger
H228	Flammable solid	Category 2	Warning

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	Aerosols		
H229	Pressurized container: may burst if heated	Category 1	Danger
H229	Pressurized container: may burst if heated	Category 2	Warning
H229	Pressurized container: may burst if heated	Category 3	Warning
	Pyrophoric gas		
H230	May react explosively even in the absence of air	1A, Chemically unstable gas A	
H231	May react explosively even in the absence of air at elevated pressure and/or temperature	1A, Chemically unstable gas B	
H232	May ignite spontaneously if exposed to air	1A, Pyrophoric gas	Danger
	Self-reactive substances and mixtures; Organic peroxides		
H240	Heating may cause an explosion	Type A	Danger
H241	Heating may cause a fire or explosion	Type B	Danger
H242	Heating may cause a fire	Type C, D	Danger
H242	Heating may cause a fire	Type E, F	Warning
	Pyrophoric liquids, Pyrophoric solids		
H250	Catches fire spontaneously if exposed to air	Category 1	Danger
	Self-heating substances and mixtures		
H251	Self-heating; may catch fire	Category 1	Danger
H252	Self-heating in large quantities; may catch fire	Category 2	Warning
	Substances and mixtures which in contact with water, emit flammable gases		
H260	In contact with water releases flammable gases which may ignite spontaneously	Category 1	Danger
H261	In contact with water releases flammable gas	Category 2	Danger
H261	In contact with water releases flammable gas	Category 3	Warning
	Oxidizing gases		
H270	May cause or intensify fire; oxidizer	Category 1	Danger
	Oxidizing liquids, Oxidizing solids		
H271	May cause fire or explosion; strong Oxidizer	Category 1	Danger
H272	May intensify fire; oxidizer	Category 2	Danger
H272	May intensify fire; oxidizer	Category 3	Warning
	Gases under pressure		

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H280	Contains gas under pressure; may explode if heated	Compressed gas, Liquefied gas, Dissolved gas	Warning
H281	Contains refrigerated gas; may cause cryogenic burns or injury	Refrigerated liquefied gas	Warning
	Chemicals under pressure		
H282	Extremely flammable chemical under pressure: may explode if heated	Category 1	Danger
H283	Flammable chemical under pressure: may explode if heated	Category 2	Warning
H284	Chemical under pressure: may explode if heated	Category 3	Warning
	Corrosive to Metals		
H290	May be corrosive to metals	Category 1	Warning

Health hazard statement

Code	**Hazard Class (GHS Chapter)**	**Hazard Category**	
	Acute toxicity, oral		
H300	Fatal if swallowed	Category 1, 2	Danger
H301	Toxic if swallowed	Category 3	Danger
H302	Harmful if swallowed	Category 4	Warning
H303	May be harmful if swallowed	Category 5	Warning
	Aspiration hazard		
H304	May be fatal if swallowed and enters airways	Category 1	Danger
H305	May be fatal if swallowed and enters airways	Category 2	Warning
	Acute toxicity, dermal		
H310	Fatal in contact with skin	Category 1, 2	Danger
H311	Toxic in contact with skin	Category 3	Danger
H312	Harmful in contact with skin	Category 4	Warning
H313	May be harmful in contact with skin	Category 5	
	Skin corrosion/irritation		
H314	Causes severe skin burns and eye damage	Category 1A, 1B, 1C	Danger
H315	Causes skin irritation	Category 2	Warning
H316	Causes mild skin irritation	Category 3	Warning

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	Sensitization, Skin		
H317	May cause an allergic skin reaction	Category 1, 1A, 1B	Warning
	Serious eye damage/eye irritation		
H318	Causes serious eye damage	Category 1	Danger
H319	Causes serious eye irritation	Category 2A	Warning
H320	Causes eye irritation	Category 2B	Warning
	Acute toxicity, inhalation		
H330	Fatal if inhaled	Category 1, 2	Danger
H331	Toxic if inhaled	Category 3	Danger
H332	Harmful if inhaled	Category 4	Warning
H333	May be harmful if inhaled	Category 5	Warning
	Sensitization, respiratory		
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled	Category 1, 1A, 1B	Danger
	Specific target organ toxicity, single exposure; Respiratory tract irritation		
H335	May cause respiratory irritation	Category 3	Warning
H336	May cause drowsiness or dizziness	Category 3	Warning
	Germ cell mutagenicity		
H340	May cause genetic defects	Category 1A, 1B	Danger
H341	Suspected of causing genetic defects	Category 2	Warning
	Carcinogenicity		
H350	May cause cancer	Category 1A, 1B	Danger
H350i	May cause cancer by inhalation	Category 1A, 1B	Danger
H351	Suspected of causing cancer	Category 2	Warning
	Reproductive toxicity		
H360	May damage fertility or the unborn child	Category 1A, 1B	Danger
H360F	May damage fertility	Category 1A, 1B	Danger
H360D	May damage the unborn child	Category 1A, 1B	Danger
H360FD	May damage fertility; May damage the unborn child	Category 1A, 1B	Danger
H360Fd	May damage fertility; Suspected of damaging the unborn child	Category 1A, 1B	Danger
H360Df	May damage the unborn child; Suspected of damaging fertility	Category 1A, 1B	Danger
H361	Suspected of damaging fertility or the unborn child	Category 2	Warning
H361f	Suspected of damaging fertility	Category 2	Warning
H361d	Suspected of damaging the unborn child	Category 2	Warning

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H361fd	Suspected of damaging fertility; Suspected of damaging the unborn child	Category 2	Warning
H362	May cause harm to breast-fed children	Additional category	
	Specific target organ toxicity, single exposure		
H370	Causes damage to organs	Category 1	Danger
H371	May cause damage to organs	Category 2	Warning
	Specific target organ toxicity, repeated exposure		
H372	Causes damage to organs through prolonged or repeated exposure	Category 1	Danger
H373	Causes damage to organs through prolonged or repeated exposure	Category 2	Warning

Environmental hazard statement

Code	**Hazard Class (GHS Chapter)**	**Hazard Category**	
	Hazardous to the aquatic environment, acute hazard		
H400	Very toxic to aquatic life	Category 1	Warning
H401	Toxic to aquatic life	Category 2	
H402	Harmful to aquatic life	Category 3	
	Hazardous to the aquatic environment, long-term hazard		
H410	Very toxic to aquatic life with long lasting effects	Category 1	Warning
H411	Toxic to aquatic life with long lasting effects	Category 2	
H412	Harmful to aquatic life with long lasting effects	Category 3	
H413	May cause long lasting harmful effects to aquatic life	Category 4	
	Hazardous to the ozone layer		
H420	Harms public health and the environment by destroying ozone in the upper atmosphere	Category 1	Warning