VLECalc 1.3 is distributed as fully functional freeware. Please use only for peaceful and legal purposes. If you have any difficulties, comments, suggestions or greetings, please send me an email!
My address is mail@vlecalc.org. I really appreciate any correspondence.

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The author will accept no liability for any use of the results provided by this program and cannot guarantee the accuracy or validity of the results. Furthermore, the author will accept no responsibility of the loss of any data or damage of any equipment or systems resulting from the use of the program. Use at your own risk.

The drop down lists in the main form of VLECalc are loaded from the first column in the Cmpd Data sheet. The order in the list will be the same as the order in the sheet. The user can reorder the Cmpd Data rows as desired, and this order does not have to be the same as the row order in the UNIFAC or the NRTL sheets.

Each of the data sets in Cmpd Data, UNIFAC and NRTL must be a continuous spreadsheet range anchored at cell A1. A blank line inserted into the range will make only those compounds above the line accessible by VLECalc to use only the compounds above the line.

DO NOT reorder the columns on any sheet. Do not add contiguous columns. Do not mix data types in columns (e.g. only put integers into the UNIFAC table.)

VLECalc looks up the information in UNIFAC and NRTL by matching the compound names. It is therefore essential that the names used in UNIFAC and NRTL sheets are identical with the names used in Cmpd Data.

For each compound, VLECalc requires that the molecular weight, density and Antoine A, B and C are entered in Cmpd Data. Tmin and Tmax are not required.

VLECalc assumes that there is a single liquid phase. It does not check for liquid phase splitting. If the system is immicisble, the estimates from VLECalc will be inaccurate.

The use of UNIFAC requires that a UNIFAC composition be defined for the compound in the UNIFAC sheet. Values of the interaction parameters are not established for all of the UNIFAC groups. VLECalc will report the occurance of a missing group interaction parameter and sets the value of that parameter to zero. It will still do the calculation, but the accuracy of the result is questionable.

An N component system requires N(N-1)/2 sets of NRTL binary interaction parameters (BIPs). Missing BIP sets will be reported by VLECalc, but NRTL will still calculate. The missing BIPs default to zero (i.e. zero interaction

will be reported by VLECalc, but NRTL will still calculate. The missing BIPs default to zero (i.e. zero interaction, an "ideal" system.) and therefore the accuracy of the result is questionable. The alpha parameter is dimensionless; $\Delta g(1,2)$ and $\Delta g(2,1)$ are in cal/mole.

When defining the binary pairs on the NRTL sheet, it does not matter which compound is taken as "1" or "2".

Antoine equation is in the form log10(Pv) = AntA - AntB/(T +AntC)
with T in Celcius. Pv is the pure component vapor pressure in mm Hg. Tmin and Tmax (Celcius) are the minimum and maximum temperature ranges for the correlation.

The values of the Antoine constants in the table are adapted from Reid, R.C., J.M. Prausnitz and T.K. Sherwood, "The Properties of Gases and Liquids", 3rd edition, McGraw Hill, 1977.

The Chemistry Data Series volume 1 "Vapor-Liquid Equilibrium Data Collection", by J. Gmehling, U. Onken and W. Arlt, published by DECHEMA, Frankfurt is an excellent source of Antoine coefficients and NRTL BIPs, and is the source of the BIPs in the table.

Unifac model parameters were taken from Vapor Liquid Equilibria by UNIFAC Group Contribution, 5. Revision and Extension. Hansen, H.K, P. Rasmussen, A. Fredenslund, M. Schiller and J Gmehling, Ind. Eng. Chem. Res. 1991, 30, 2355-2358

	MWT (g/mol)	Density (Kg/Lit)	AntA	AntB	AntC	Tmin (C)	Tmax (C)
1,2-Dimethoxyethane	90.12	0.867	6.95918	1246.33	220.00	-11	120
2,2,4-Trimethylpentane	114.23	0.692	6.81191	1257.84	220.74	-4	125
Acetaldehyde	44.05	0.778	7.05646	1070.60	236.00	-63	47
Acetic Acid	60.05	1.049	7.29962	1479.02	216.81	17	157
Acetic Anhydride	102.09	1.087	7.12165	1427.77	198.04	35	164
Acetone	58.08	0.790	7.23157	1277.09	237.22	-32	77
Acetonitrile	41.05	0.782	7.07353	1279.20	224.00	-13	117
Acetylene	26.04	0.615	7.09989	711.00	253.38	-79	-71
Ammonia	17.03	0.639	7.36047	926.13	240.17	-94	-12
Aniline	93.13	1.022	7.24177	1675.30	200.00	67	227
Benzaldehyde	106.12	1.045	7.10076	1628.00	207.03	27	187
Benzene	78.11	0.885	6.90563	1211.03	220.79	7	104
Benzyl Alcohol	108.14	1.041	7.58200	1904.30	200.00	112	330
Bromobenzene	157.01	1.495	6.86064	1438.82	205.44	47	177
Butane	58.12	0.579	6.80896	935.86	238.73	-78	17
Chlorobenzene	112.56	1.106	6.97807	1431.05	217.55	47	147
Diethylamine	73.14	0.707	6.97238	1127.00	220.00	-31	77
Diisopropyl Ether	102.18	0.724	7.09711	1257.60	230.00	-24	91
Dimethylamine	45.09	0.656	7.06393	1024.40	238.00	-55	37
Ethyl Acetate	88.11	0.901	7.01455	1211.90	216.00	-13	112
Ethyl Alcohol	46.07	0.789	8.21333	1652.05	231.47	-3	96
Ethyl Ether	74.12	0.713	6.98467	1090.64	231.20	-48	67
Ethyl Formate	74.08	0.927	7.01868	1130.60	219.00	-33	87
Ethylamine	45.09	0.683	7.38618	1137.30	235.85	-58	43
Ethylene Glycol	62.07	1.114	8.79451	2615.40	244.90	91	221
Formaldehyde	30.03	0.815	7.15609	957.24	243.00	-88	-2
Formic Acid	46.03	1.226	7.37788	1563.28	247.06	-2	136
Isobutane	58.12	0.557	6.74811	882.80	240.00	-86	7
Isobutyl Alcohol	74.12	0.802	7.32707	1248.48	172.85	20	15
Isopropyl Alcohol	60.10	0.786	8.11822	1580.92	219.61	0	101
Isopropyl Chloride	78.54	0.862	6.96539	1081.60	230.00	-48	67
Isopropylamine	59.11	0.688	7.10666	1121.50	233.00	-34	64
Methane	16.04	0.425	6.61183	389.93	265.99	-180	-153
Methanol	32.04	0.791	8.07245	1574.99	238.86	-16	91
Methyl Acetate	74.08	0.934	7.00495	1130.00	217.00	-28	87
Methyl Ethyl Ketone	72.11	0.805	7.20790	1368.21	236.50	-16	103
Methyl Isobutyl Ketone	100.16	0.801	6.82559	1256.70	202.40	12	152
Methylamine	31.06	0.703	7.49688	1079.15	240.23	-61	38
Methylene Chloride	84.93	1.317	7.08026	1138.91	231.45	-44	59
m-Xylene	106.17	0.864	7.00908	1462.27	215.11	27	167
n-Butyl Acetate	116.16	0.898	7.02845	1368.50	204.00	22	162
n-Butyl Alcohol	74.12	0.810	7.47681	1362.39	178.72	15	131
n-Butylamine	73.14	0.739	7.21298	1308.40	224.19	-14	100
n-Heptane	100.21	0.684	6.89386	1264.37	216.64	-3	127
n-Hexane	86.18	0.659	6.87775	1171.53	224.37	-28	97
Nitromethane	61.04	1.138	7.04395	1291.00	209.00	5	136
n-Octane	114.23	0.703	6.92378	1355.12	209.52	19	152

	MWT (g/mol)	Density (Kg/Lit)	AntA	AntB	AntC	Tmin (C)	Tmax (C)
n-Pentane	72.15	0.626	6.87631	1075.78	233.21	-53	57
n-Propyl Alcohol	60.10	0.804	7.61922	1375.14	193.00	12	127
n-Propyl Acetate	102.13	0.887	7.04821	1294.40	209.00	7	137
n-Propyl Chloride	78.54	0.891	6.93108	1121.12	230.20	-43	77
n-Propylamine	59.11	0.717	6.94684	1108.20	224.00	-38	77
o-Dichlorobenzene	147.00	1.306	7.07027	1649.55	213.31	58	210
o-Xylene	106.17	0.880	6.99892	1474.68	213.69	32	172
Piperidine	85.15	0.862	6.99231	1309.60	212.00	7	143
Propane	44.10	0.582	6.82972	813.20	247.99	-109	-24
p-Xylene	106.17	0.861	6.99053	1453.43	215.31	27	167
Pyridine	79.10	0.983	6.98823	1344.20	212.00	12	152
sec-Butyl Alcohol	74.12	0.807	7.47429	1314.19	186.50	25	120
tert-Butyl Alcohol	74.12	0.787	7.31995	1154.48	177.65	20	103
Tetrahydrofuran	72.11	0.889	6.99514	1202.29	226.25	-3	97
Toluene	92.14	0.867	6.95466	1344.80	219.48	7	137
Triethylamine	101.19	0.728	6.89890	1251.80	222.00	-13	127
Trimethylamine	59.11	0.633	6.97038	968.70	234.00	-58	32
Water	18.02	0.998	7.94915	1657.46	227.02	11	168

	Alkane				Alkene					Aromatic					Alcohol				Ketone		Aldehyde	Ester			Ether				Amine, 1st		
	CH3	CH2	CH	C	CH2=CH	CH=CH	CH2=C	CH=C	C=C	ACH	AC	ACCH3	ACCH2	ACCH	OH	CH3OH	H2O	ACOH	CH3CO	CH2CO	CHO	CH3COO	CH2COO	HCOO	CH3O	CH2O	CH-O	FCH2O	CH3NH2	CH2NH2	CHNH2
1,2-Dimethoxyethane		2																							2						
2,2,4-Trimethylpentane	5	1	1	1																											
Acetaldehyde	1																				1										
Acetic Acid	1																														
Acetone	1																		1												
Acetonitrile																															
Aniline										5																					
Benzaldehyde										5	1										1										
Benzene										6																					
Benzyl Alcohol										5			1		1																
Bromobenzene										5	1																				
Butane	2	2																													
Chlorobenzene										5																					
Diethylamine	2	1																													
Diisopropylamine	4		1																												
Dimethyl Sulfoxide																															
Dimethylamine	1																														
Ethyl Acetate	1	1																				1									
Ethyl Alcohol	1	1													1																
Ethyl Ether	2	1																								1					
Ethyl Formate	1	1																						1							
Ethylamine	1																													1	
Ethylene Glycol																															
Formic Acid																															
Isobutane	3		1																												
Isobutyl Alcohol	2	1	1												1																

	Alkane				Alkene					Aromatic					Alcohol				Ketone		Aldehyde	Ester			Ether				Amine, 1st		
	CH3	CH2	CH	C	CH2=CH	CH=CH	CH2=C	CH=C	C=C	ACH	AC	ACCH3	ACCH2	ACCH	OH	CH3OH	H2O	ACOH	CH3CO	CH2CO	CHO	CH3COO	CH2COO	HCOO	CH3O	CH2O	CH-O	FCH2O	CH3NH2	CH2NH2	CHNH2
Isopropyl Acetate	2		1																			1									
Isopropyl Alcohol	2		1												1																
Methanol																1															
Methyl Acetate	1																					1									
Methylamine																													1		
Methyl Ethyl Ketone	1	1																	1												
Methyl Formate	1																							1							
Methyl Isobutyl Ketone	2	1	1																1												
Methyl tert-Butyl Ether	3			1																					1						
Methylene Chloride																															
N,N-Dimethyl Formamide																															
n-Butyl Acetate	1	3																				1									
n-Butyl Alcohol	1	3													1																
n-Butylamine	1	2																												1	
n-Butyl Chloride	1	2																													
n-Heptane	2	5																													
n-Hexane	2	4																													
n-Pentane	2	3																													
n-Propyl Alcohol	1	2													1																
o-Dichlorobenzene										4																					
o-Xylene										4		2																			
Piperidine		4																													
n-Propyl Acetate	1	2																				1									
Propane	2	1																													
Pyridine																															
sec-Butyl Alcohol	2	1	1												1																

	Alkane				Alkene					Aromatic					Alcohol				Ketone		Aldehyde	Ester			Ether				Amine, 1st		
	CH3	CH2	CH	C	CH2=CH	CH=CH	CH2=C	CH=C	C=C	ACH	AC	ACCH3	ACCH2	ACCH	OH	CH3OH	H2O	ACOH	CH3CO	CH2CO	CHO	CH3COO	CH2COO	HCOO	CH3O	CH2O	CH-O	FCH2O	CH3NH2	CH2NH2	CHNH2
tert-Butyl Alcohol	3			1											1															
Tetrahydrofuran		3																										1			
Toluene										5		1																			
Triethylamine	3	2																													
Trimethylamine	2																														
Water																	1														

	Amine, 2nd			Amine, 3rd		Aniline	Pyridine			Nitrile		Acid		Chloride			Dichloride			Other Chloride				Nitro					Thiol		
	CH3NH	CH2NH	CHNH	CH3N	CH2N	ACNH2	C5H5N	C5H4N	C5H3N	CH3CN	CH2CN	COOH	HCOOH	CH2Cl	CHCl	CCl	CH2Cl2	CHCl2	CCl2	CHCl3	CCl3	CCl4	ACCl	CH3NO2	CH2NO2	CHNO2	ACNO2	CS2	CH3SH	CH2SH	furfural
1,2-Dimethoxyethane																															
2,2,4-Trimethylpentane																															
Acetaldehyde																															
Acetic Acid												1																			
Acetone																															
Acetonitrile										1																					
Aniline						1																									
Benzaldehyde																															
Benzene																															
Benzyl Alcohol																															
Bromobenzene																															
Butane																															
Chlorobenzene																							1								
Diethylamine		1																													
Diisopropylamine			1																												
Dimethyl Sulfoxide																															
Dimethylamine	1																														
Ethyl Acetate																															
Ethyl Alcohol																															
Ethyl Ether																															
Ethyl Formate																															
Ethylamine																															
Ethylene Glycol																															
Formic Acid													1																		
Isobutane																															
Isobutyl Alcohol																															

	Amine, 2nd			Amine, 3rd		Aniline	Pyridine			Nitrile		Acid		Chloride			Dichloride			Other Chloride				Nitro					Thiol		
	CH3NH	CH2NH	CHNH	CH3N	CH2N	ACNH2	C5H5N	C5H4N	C5H3N	CH3CN	CH2CN	COOH	HCOOH	CH2Cl	CHCl	CCl	CH2Cl2	CHCl2	CCl2	CHCl3	CCl3	CCl4	ACCl	CH3NO2	CH2NO2	CHNO2	ACNO2	CS2	CH3SH	CH2SH	furfural
Isopropyl Acetate																															
Isopropyl Alcohol																															
Methanol																															
Methyl Acetate																															
Methylamine																															
Methyl Ethyl Ketone																															
Methyl Formate																															
Methyl Isobutyl Ketone																															
Methyl tert-Butyl Ether																															
Methylene Chloride																	1														
N,N-Dimethyl Formamide																															
n-Butyl Acetate																															
n-Butyl Alcohol																															
n-Butylamine																															
n-Butyl Chloride														1																	
n-Heptane																															
n-Hexane																															
n-Pentane																															
n-Propyl Alcohol																															
o-Dichlorobenzene																							2								
o-Xylene																															
Piperidine		1																													
n-Propyl Acetate																															
Propane																															
Pyridine							1																								
sec-Butyl Alcohol																															

	Amine, 2nd			Amine, 3rd		Aniline	Pyridine			Nitrile		Acid		Chloride			Dichloride			Other Chloride				Nitro					Thiol		
	CH3NH	CH2NH	CHNH	CH3N	CH2N	ACNH2	C5H5N	C5H4N	C5H3N	CH3CN	CH2CN	COOH	HCOOH	CH2Cl	CHCl	CCl	CH2Cl2	CHCl2	CCl2	CHCl3	CCl3	CCl4	ACCl	CH3NO2	CH2NO2	CHNO2	ACNO2	CS2	CH3SH	CH2SH	furfural
tert-Butyl Alcohol																														
Tetrahydrofuran																														
Toluene																														
Triethylamine					1																									
Trimethylamine				1																										
Water																														

		iodo	bromo	alkyne						Formamide		Fluorides			Flexy Ester	Silane				Siloxane				Chlorofluorocarbons							
	(CH2OH)2	I	Br	CH=-C	C=-C	DMSO	ACRY	Cl-(C=C)	ACF	DMF-1	DMF-2	CF3	CF2	CF	COO	SiH3	SiH2	SiH	Si	SiH2O	SiHO	SiO	NMP	CCl3F	CCl2F	HCCl2F	HCClF	CClF2	HCClF2	CClF3	CCl2F2
1,2-Dimethoxyethane																															
2,2,4-Trimethylpentane																															
Acetaldehyde																															
Acetic Acid																															
Acetone																															
Acetonitrile																															
Aniline																															
Benzaldehyde																															
Benzene																															
Benzyl Alcohol																															
Bromobenzene			1																												
Butane																															
Chlorobenzene																															
Diethylamine																															
Diisopropylamine																															
Dimethyl Sulfoxide						1																									
Dimethylamine																															
Ethyl Acetate																															
Ethyl Alcohol																															
Ethyl Ether																															
Ethyl Formate																															
Ethylamine																															
Ethylene Glycol	1																														
Formic Acid																															
Isobutane																															
Isobutyl Alcohol																															

		iodo	bromo	alkyne						Formamide		Fluorides			Flexy Ester	Silane				Siloxane				Chlorofluorocarbons							
	(CH2OH)2	I	Br	CH=-C	C=-C	DMSO	ACRY	Cl-(C=C)	ACF	DMF-1	DMF-2	CF3	CF2	CF	COO	SiH3	SiH2	SiH	Si	SiH2O	SiHO	SiO	NMP	CCl3F	CCl2F	HCCl2F	HCClF	CClF2	HCClF2	CClF3	CCl2F2
Isopropyl Acetate																															
Isopropyl Alcohol																															
Methanol																															
Methyl Acetate																															
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Methyl Ethyl Ketone																															
Methyl Formate																															
Methyl Isobutyl Ketone																															
Methyl tert-Butyl Ether																															
Methylene Chloride																															
N,N-Dimethyl Formamide										1																					
n-Butyl Acetate																															
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n-Butyl Chloride																															
n-Heptane																															
n-Hexane																															
n-Pentane																															
n-Propyl Alcohol																															
o-Dichlorobenzene																															
o-Xylene																															
Piperidine																															
n-Propyl Acetate																															
Propane																															
Pyridine																															
sec-Butyl Alcohol																															

	Amides						Glycol Ethers		Sulfides				
	CONH2	CONHCH3	CONHCH2	CON(CH3)2	CONCH3CH2	CON(CH2)2	C2H5O2	C2H4O2	CH3S	CH2S	CHS	Morpholine	Thiophene
1,2-Dimethoxyethane													
2,2,4-Trimethylpentane													
Acetaldehyde													
Acetic Acid													
Acetone													
Acetonitrile													
Aniline													
Benzaldehyde													
Benzene													
Benzyl Alcohol													
Bromobenzene													
Butane													
Chlorobenzene													
Diethylamine													
Diisopropylamine													
Dimethyl Sulfoxide													
Dimethylamine													
Ethyl Acetate													
Ethyl Alcohol													
Ethyl Ether													
Ethyl Formate													
Ethylamine													
Ethylene Glycol													
Formic Acid													
Isobutane													
Isobutyl Alcohol													

Cmpd(1)	Cmpd(2)	Δg(1,2) (cal/mol)	Δg(2,1) (cal/mol)	α(1,2)
Methanol	Water	-253.8802	845.2062	0.2994
Acetonitrile	Water	364.8365	1321.7321	0.2858
Water	Acetic Acid	712.1791	320.1059	1.4032
Ethyl Alcohol	Water	-109.6339	1332.3134	0.3031
Acetone	Water	628.2471	1198.1984	0.5341
Water	N,N-Dimethylformamid	667.6168	-339.4763	0.3041
n-Propyl Alcohol	Water	500.3962	1636.572	0.5081
Isopropyl Alcohol	Water	-26.279	1569.2943	0.2879
Methyl Ethyl Ketone	Water	674.4614	1809.8868	0.3536
Tetrahydrofuran	Water	915.745	1725.0977	0.4522
Ethyl Acetate	Water	935.688	2316.3631	0.4104
Water	n-Butyl Alcohol	2633.6951	504.0381	0.4447
Isobutyl Alcohol	Water	231.363	2388.5153	0.4027
tert-Butyl Alcohol	Water	419.1944	2096.6985	0.5007
Diethylamine	Water	-169.1652	1372.3121	0.2932
Water	Pyridine	1835.0881	419.8087	0.6802
Water	n-Butyl Acetate	3805.0038	918.2419	0.2951
Diisopropylamine	Water	899.0145	1842.5789	0.5395
Triethylamine	Water	2058.3746	2072.9748	0.4144
Acetaldehyde	Water	1034.0769	310.5491	0.2878
Ethylene Glycol	Water	43.4737	-22.8913	0.3056
Dimethylamine	Water	-615.7161	518.7112	0.3062