Mc Cabe – Thiele

PARA DESTILACIÓN DE MEZCLAS BINARIAS

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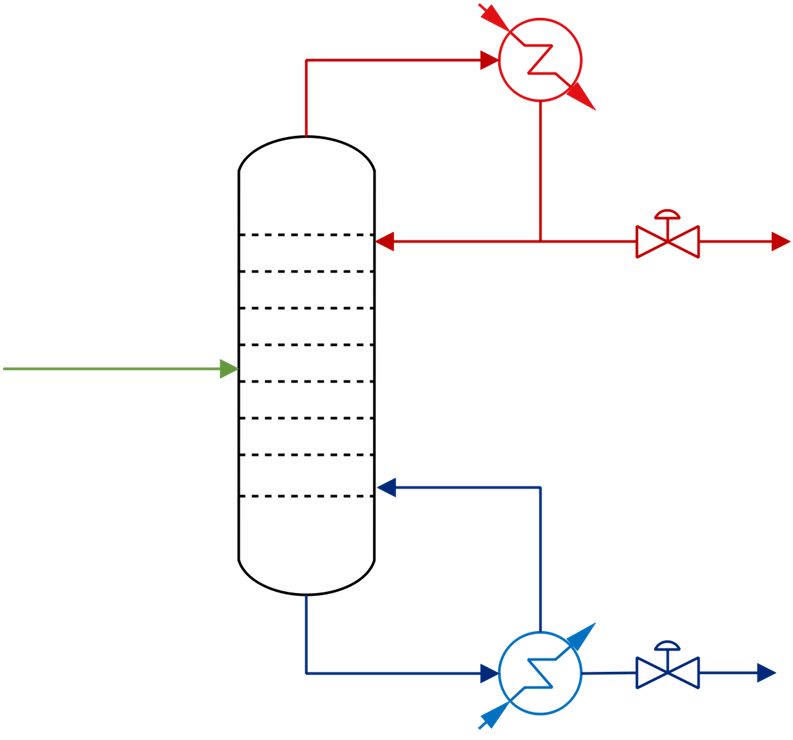
SMath Studio 0.99 / @ Presión Constante



Realiza con facilidad las siguientes tareas:

Gráficos

- Temperatura vs Composición
- Presión de saturación 1 vs Composición
- Presión de saturación 2 vs Composición
- Composición x vs Composición y
- Gráfico McCabe Thiele para Etapas mínimas
- Gráfico McCabe Thiele para Etapas Requeridas

Tablas

- Resultados del Equilibrio del sistema binario LV
- Coordenadas del punto pinch
- Coordenada de la intercepción de la línea de rectificación con la de agotamiento
- Coordenadas de los puntos de las etapas requeridas del diagrama McCabe

Y mucho más.

Iztapalapa Ciudad de México 2020

"Water"	8.0713	1730.63	233.426	1	100	99.9968
"carbon−tetrachloride"	6.8941	1219.58	227.17	− 20	101	76.7156
"trichlorofluoromethane"	6.8843	1043.01	236.86	− 33	27	23.6654
"dichlorodifluoromethane"	6.6862	782.072	235.377	− 119	− 30	− 29.8594
"chlorotrifluoromethane"	6.3511	522.061	231.677	− 150	− 81	− 81.2391
"carbon−tetrafluoride"	6.9723	540.5	260.1	− 180	− 125	− 127.9964
"carbon−monoxide"	6.2402	230.27	260.01	− 210	− 165	− 191.4647
"carbon−dioxide"	9.8106	1347.79	273	− 119	− 69	− 78.5077
"carbonyl−sulfide"	6.9072	804.48	250	− 111	− 49	− 50.1995
"carbon−disulfide"	6.9419	1168.62	241.54	− 45	69	46.2204
"chloroform"	6.9371	1171.2	227	− 13	97	61.737
"dichlorofluoromethane"	6.9758	996.267	234.172	− 91	9	9.1204
"chlorodifluoromethane"	6.7577	740.39	231.86	− 48	− 33	− 40.8846
"trifluoromethane"	7.0886	705.33	249.78	− 128	− 82	− 82.155
"triiodomethane"	6.596	1567.8	204	137	254	217.9999
"dichloromethane"	7.0803	1138.91	231.46	− 44	59	39.7422
"chlorofluoromethane"	6.2045	740.39	231.86	− 55	12	− 9.0997
"difluoromethane"	7.1389	821.7	244.7	− 82	− 32	− 51.726
"diiodomethane"	6.9425	1567.8	204	83	232	182.0011
"formaldehyde"	7.1561	957.24	243.01	− 88	− 2	− 19.1092
"formic−acid"	7.3779	1563.28	247.07	− 2	136	100.5506
"bromomethane"	6.9597	986.59	238.33	− 58	53	3.5473
"chloromethane"	6.9944	902.45	243.61	− 93	− 7	− 24.2272
"fluoromethane"	7.0976	740.22	253.89	− 132	− 64	− 78.3487
"iodomethane"	6.988	1146.34	236.66	− 13	52	42.4459
"nitromethane"	7.044	1291	209.01	5	136	101.089
"methane"	6.6956	405.42	267.777	− 181	− 152	− 161.5013
"methanol"	8.0724	1574.99	238.87	− 16	91	64.5036
"methanethiol"	7.0316	1015.547	238.706	− 70	25	5.956
"methylamine"	7.4969	1079.15	240.24	− 61	38	− 6.4597
"tetrachloroethene"	7.02	1415.49	221.01	34	187	120.963
"hexachloroethane"	7.0863	1626.945	197.048	33	186	189.8117
"1,1,2−trichlorotrifluoroethane"	6.8803	1099.9	227.5	− 25	83	47.5103
"1,2−dichlorotetrafluoroethane"	6.8708	942.336	232.632	− 95	4	3.5409
"chloropentafluoroethane"	6.8333	802.97	242.28	− 98	− 43	− 39.1243
"tetrafluoroethene"	6.8966	683.84	245.94	− 133	− 63	− 75.6521
"hexafluoroethane"	6.7933	657.06	246.22	− 103	− 73	− 78.2808
"cyanogen"	6.4363	576.579	182.308	− 77	− 4	− 20.1415
"trichloroethene"	7.0281	1315.1	230.01	− 13	127	87.0889
"pentachloroethane"	6.74	1378	197	25	162	160.0701
"trifluoroethene"	5.6872	491.359	227.23	− 93	− 31	− 52.1409
"acetylene(ethyne)"	9.1402	1232.6	280.9	− 129	− 83	− 83.9797
"1,1−dichloroethene"	6.9722	1099.4	237.2	− 28	32	31.5109
"cis−1,2−dichloroethene"	7.0223	1205.4	230.6	0	84	60.4549
"trans−1,2−dichloroethene"	6.9651	1141.9	231.9	− 38	85	47.6837
"1,1,2,2−tetrachloroethane"	6.6317	1228.1	179.9	25	130	147.5159
"1,1−difluoroethene"	6.3492	491.359	227.239	− 140	− 86	− 85.5703
"cis−1,2−difluoroethene"	5.314	491.359	227.23	− 78	2.6	− 25.2903
"trans−1,2−difluoroethene"	5.314	491.359	227.23	− 78	2.6	− 25.2903
"ketene"	6.9573	803.1	238.01	− 103	− 18	− 41.0021
"bromoethylene"	7.2438	1219.308	264.021	− 88	16	15.446

"chloroethene"	6.4971	783.4	230.01	− 88	17	− 13.3789
"1,1,2−trichloroethane"	6.9653	1351	217	29	155	113.7637
"acetyl−chloride"	6.8407	1062.86	217.63	− 36	82	50.7767
"fluoroethene"	6.3395	593.551	243.111	− 149	− 72	− 71.4988
"1,1,1−trifluoroethane"	6.9038	788.21	243.24	− 3	27	− 47.3134
"acetonitrile"	7.0735	1279.2	224.01	− 13	117	81.0927
"ethylene"	6.7476	585	255	− 153	− 91	− 103.71
"1,2−dibromoethane"	6.7215	1280.82	201.75	52	131	131.739
"1,1−dichloroethane"	6.9853	1171.42	228.13	− 31	79	57.2699
"1,2−dichloroethane"	7.0253	1271.25	222.94	− 33	100	83.7928
"1,1−difluoroethane"	7.03	910	244	− 35	0	− 24.6799
"1,2−diiodoethane"	6.9883	1647.1	201	98	253	199.9956
"ethylene−oxide"	7.2701	1115.1	244.15	− 73	37	9.9004
"acetaldehyde"	7.0565	1070.6	236.01	− 63	47	20.379
"acetic−acid"	7.2996	1479.02	216.82	17	157	117.8918
"methyl−formate"	7.1704	1125.2	230.56	− 48	51	31.7497
"thioacetic−acid"	7.7489	1479.02	216.82	40	106	87.0002
"thiacyclopropane"	7.0372	1194.37	232.42	− 35	77	54.9343
"bromoethane"	6.92	1090.81	231.72	− 47	60	38.3369
"chloroethane"	6.94	1012.78	236.68	− 73	37	12.8232
"fluoroethane"	6.9785	854.21	246.16	− 103	− 21	− 37.6985
"iodoethane"	6.959	1232	229	30	60	73.0951
"ethylenimine"	7.1323	1133.7	210.01	− 25	86	56.6497
"nitroethane"	7.5878	1671.266	241.187	− 21	114	113.876
"ethyl−nitrate"	7.1637	1338.8	224.9	0	60	87.6929
"ethane"	6.8345	663.7	256.47	− 143	− 75	− 88.6022
"methyl−ether"	7.3164	1025.56	256.06	− 94	− 8	− 24.8482
"ethyl−alcohol"	8.2133	1652.05	231.48	− 3	96	78.3286
"ethylene−glycol"	8.7945	2615.4	244.91	91	221	197.3522
"methyl−sulfide"	6.9488	1090.755	230.799	− 47	58	37.3331
"ethanethiol"	6.9521	1084.531	231.385	− 49	56	35.003
"methyl−disulfide"	6.9779	1346.342	218.863	6	135	109.745
"ethylamine"	7.3862	1137.3	235.86	− 58	43	16.5712
"dimethylamine"	7.0639	1024.4	238.01	− 55	37	6.8809
"acrylonitrile"	6.9163	1208.3	222.01	− 18	112	77.4087
"allene(propadiene)"	5.7137	458.06	196.07	− 99	− 16	− 34.3763
"propyne(methylacetylene)"	6.7848	803.73	229.08	− 90	− 6	− 23.2085
"acrylic−acid"	7.1926	1441.5	193.01	42	177	141.3062
"3−bromo−1−propene"	7.0519	1259.83	232.04	17	93	70.001
"3−chloro−1−propene"	6.9388	1099.6	226.01	− 43	77	44.9618
"1,2,3−trichloropropane"	7.0028	1484.1	204.01	42	197	156.0349
"3−iodo−1−propene"	6.9693	1316.5	220	20	142	102.0018
"propionitrile"	6.9301	1277.2	218.01	− 3	132	97.4036
"propene"	6.8196	785	247	− 112	− 32	− 47.7
"cyclopropane"	6.8879	856.01	246.51	− 93	− 28	− 32.886
"1,2−dibromopropane"	6.891	1419.6	212	50	250	141.9941
"1,2−dichloropropane"	6.9654	1296.4	221	15	135	96.3883
"1,3−dichloropropane"	6.9719	1376.2	216	34	162	120.3932
"2,2−dichloropropane"	6.9482	1201.1	226	− 6	105	69.3002
"1,2−diiodopropane"	6.0765	1507.41	244.7	125	275	227.0015
"propylene−oxide"	6.6546	915.31	208.29	− 48	67	34.2542
"allyl−alcohol"	7.3424	1271.7	188.01	13	127	97.0231
"propionaldehyde"	7.0493	1154.8	229.01	− 38	77	48.021
"acetone"	7.2316	1277.03	237.23	− 32	77	56.2871
"thiacyclobutane"	7.0167	1321.331	224.513	− 5	120	94.9688
"1−bromopropane"	7.0377	1259.836	232.042	− 53	71	71.0329

"2−bromopropane"	7.0046	1223.475	236.508	− 62	60	60.1771
"1−chloropropane"	6.9311	1121.12	230.21	− 43	77	46.5902
"2−chloropropane"	6.9654	1081.6	230.01	− 48	67	34.7904
"1−fluoropropane"	6.9533	965.18	239.5	− 70	30	− 2.4998
"2−fluoropropane"	7.0745	965.18	239.5	− 49	8	− 9.3498
"1−iodopropane"	7.2212	1507.41	244.701	− 36	103	102.5968
"2−iodopropane"	7.0167	1340.448	234.365	− 43	90	89.7367
"1−nitropropane"	7.1146	1467.45	215.23	59	131	131.3746
"2−nitropropane"	7.4865	1664.036	240.995	− 19	120	120.3022
"propyl−nitrate"	7.7372	1721.723	245.49	0	70	109.0383
"isopropyl−nitrate"	6.4201	1018.568	183.528	0	70	104.2643
"propane"	6.804	803.81	246.99	− 108	− 25	− 42.1019
"ethyl−methyl−ether"	5.8819	504.49	160.76	− 68	37	7.3425
"propyl−alcohol"	7.6192	1375.14	193.01	12	127	97.2027
"isopropyl−alcohol"	8.1182	1580.92	219.62	0	101	82.2328
"ethyl−methyl−sulfide"	6.9385	1182.562	224.784	− 26	90	66.6542
"1−propanethiol"	6.9285	1183.307	224.624	− 25	91	67.7205
"2−propanethiol"	6.8773	1113.895	226.157	− 37	75	52.5588
"propylamine"	6.9468	1108.2	224.01	− 38	77	48.5438
"trimethylamine"	6.9704	968.7	234.01	− 58	32	2.8599
"octafluorocyclobutane"	6.8153	862.49	225.15	− 32	1	− 5.9371
"butadiyne(biacetylene)"	5.5192	460.684	164.594	− 78	0	10.0162
"1buten3yne(vinylacetylene)"	6.953	957	230.01	− 73	32	4.9989
"furan"	6.9753	1060.85	227.75	− 35	90	31.3423
"thiophene"	6.9593	1246.02	221.35	− 12	108	84.1634
"1,2−butadiene"	6.9938	1041.117	242.274	− 26	30	10.8534
"1,3−butadiene"	6.85	930.546	238.854	− 58	14	− 4.4109
"1−butyne(ethylacetylene)"	6.982	988.75	233.01	− 68	27	8.0799
"2−butyne(dimethylacetylene)"	7.0734	1101.71	235.81	− 30	47	26.967
"cyclobutene"	6.9577	1009.32	244.986	− 77	2	2.5859
"acetic−anhydride"	7.1216	1427.77	198.05	35	164	138.6258
"butyronitrile"	7.0396	1390.7	217	34	160	117.4004
"isobutyronitrile"	7.2159	1390.7	217	49	127	103.8002
"1−butene"	6.8429	926.1	240	− 81	13	− 6.2595
"2−butene,cis"	6.8693	960.1	237	− 73	23	3.7203
"2−butene,trans"	6.8695	960.8	240	− 76	20	0.8801
"2−methylpropene"	6.8413	923.2	240	− 82	12	− 6.8997
"cyclobutane"	6.9163	1024.54	241.38	− 73	17	12.5027
"1,2−dibromobutane"	7.257	1759.076	235.009	8	166	166.9602
"2,3−dibromobutane"	7.2002	1691.481	230.223	5	161	161.3764
"1,2−diiodobutane"	6.2433	1507.41	244.7	110	246	203.6022
"butyraldehyde"	7.0212	1233	223.01	− 18	107	74.7883
"2−butanone"	7.2087	1368.21	236.51	− 16	103	79.6281
"p−dioxane"	7.0063	1288.5	211.01	2	137	101.3168
"ethyl−acetate"	7.0146	1211.9	216.01	− 13	112	77.1595
"thiacyclopentane"	6.9954	1401.939	219.607	14	147	121.1172
"1−bromobutane"	6.9225	1298.608	219.7	19	141	101.6003
"2−bromobutane"	6.8272	1229.08	220	10	146	91.4413
"2−bromo−2−methylpropane"	6.6685	1129.7	225	− 7	110	73.2559
"1−chlorobutane"	6.9379	1227.43	224.11	− 18	112	78.4298
"2−chlorobutane"	6.9447	1195.8	226.01	− 23	102	68.2404
"1−chloro−2−methylpropane"	6.953	1205.079	227.046	− 54	69	68.8803
"2−chloro−2−methylpropane"	6.8671	1114.9	229.01	− 38	87	50.6739
"2−iodo−2−methylpropane"	7.2539	1507.41	244.7	42	124	100.0016
"pyrrolidine"	6.9246	1179.99	205.26	27	127	86.5432
"1−nitrobutane"	6.8672	1467.45	215.23	86	182	152.89
"2−nitrobutane"	7.252	1664.03	240.99	75	167	139.6942

"butane"	6.809	935.86	238.73	−78	19	−0.4853
"2−methylpropane(isobutane)"	6.9105	946.35	246.68	−87	7	−11.8343
"ethyl−ether"	6.9203	1064.07	228.8	−61	20	34.6158
"methyl−propyl−ether"	6.1186	708.69	179.9	0	39	38.981
"methyl−isopropyl−ether"	6.245	708.69	179.9	−12	51	30.7603
"butyl−alcohol"	7.4768	1362.39	178.73	15	131	117.7004
"sec−butyl−alcohol"	7.4743	1314.19	186.51	25	120	99.5886
"tert−butyl−alcohol"	7.3199	1154.48	177.66	20	103	82.4115
"ethylsulfide"	6.9284	1257.833	218.662	−6	117	92.1023
"isopropyl−methyl−sulfide"	6.902	1232.17	221.67	−13	109	84.7526
"methyl−propyl−sulfide"	6.9554	1284.32	219.66	−4	120	95.5387
"1−butanethiol"	6.9275	1281.018	218.1	−2	123	98.4566
"2−butanethiol"	6.887	1229.904	222.021	−13	109	84.9817
"2−methyl−1−propanethiol"	6.8875	1237.282	220.313	−10	113	88.4944
"2−methyl−2−propanethiol"	6.7878	1115.565	221.314	1	87	64.2161
"ethyl−disulfide"	6.9751	1485.97	208.958	40	182	153.9821
"butylamine"	7.213	1308.4	224.2	−14	100	77.8184
"sec−butylamine"	7.1507	1238.3	227	−9	98	63.0084
"tert−butylamine"	6.7831	993.262	210.493	19	75	44.041
"diethylamine"	6.9724	1127	220.01	−31	77	55.4333
"pyridine"	6.9882	1344.2	212.01	12	152	115.2541
"2−methylthiophene"	6.939	1326.48	214.31	9	138	112.5576
"3−methylthiophene"	6.9861	1363.84	216.78	11	141	115.4347
"1,2−pentadiene"	6.9182	1104.991	228.851	−20	66	44.8387
"1,3−pentadiene,cis"	6.9109	1101.923	229.367	−17	65	44.0578
"1,3−pentadiene,trans"	6.9132	1103.84	231.724	−16	63	42.0216
"1,4−pentadiene"	6.8354	1017.995	231.461	−33	46	25.9584
"2,3−pentadiene"	6.9622	1126.837	227.841	−13	69	48.2534
"3−methyl−1,2−butadiene"	6.9435	1103.901	230.89	−20	62	40.827
"2−methyl−1,3−butadiene"	6.8856	1071.578	233.513	−18	55	34.0586
"1−pentyne"	6.9673	1092.52	227.19	−43	62	40.1595
"2−pentyne"	7.0461	1189.87	229.6	−33	78	56.0607
"3−methyl−1−butyne"	6.8848	1014.81	227.11	−55	47	26.3399
"cyclopentene"	6.9207	1121.81	233.46	−29	105	44.2236
"spiropentane"	6.917	1090.08	231.1	3	71	38.9767
"1−pentene"	6.8465	1044.895	233.516	−55	51	29.968
"2−pentene,cis"	6.8727	1067.951	230.585	−49	58	36.9427
"2−pentene,trans"	6.9058	1083.987	232.965	−49	58	36.3528
"2−methyl−1−butene"	6.8731	1053.78	232.788	−53	52	31.1634
"3−methyl−1−butene"	6.8262	1013.474	236.816	−63	41	20.061
"2−methyl−2−butene"	6.9156	1095.088	232.842	−48	60	38.5683
"cyclopentane"	6.8868	1124.162	231.361	−40	72	49.2623
"2,3−dibromo−2−methylbutane"	7.3674	1695.9	207	81	218	170.9976
"valeraldehyde"	7.0192	1316	215.01	4	139	102.9883
"2−pentanone"	6.95	1274.6	210.91	2	137	102.3221
"thiacyclohexane"	6.9052	1422.47	211.72	29	170	141.7443
"cyclopentanethiol"	6.915	1388.63	212.05	81	173	132.1682
"1−bromopentane"	6.9558	1401.634	214.38	41	173	129.5804
"1−chloropentane"	6.9662	1332.89	218.5	24	148	107.7604
"1−chloro−3−methylbutane"	6.7953	1258.5	223	39	124	98.5006
"2−chloro−2−methylbutane"	6.959	1258.5	223	7	123	85.5915
"pentane"	6.8763	1075.78	233.205	−50	58	36.0425
"2−methylbutane(isopentane)"	6.8332	1040.73	235.445	−57	49	27.8752
"2,2−dimethypropane"	6.6043	883.42	227.782	−13	29	9.476
"methyl−tert−butyl−ether"	5.896	708.69	179.9	2	80	55.1402
"pentyl−alcohol"	7.1776	1314.56	168.16	37	138	137.7803

"tert–pentyl–alcohol"	7.8753	1604.7	208.16	55	133	113.1343
"butyl–methyl–sulfide"	6.9458	1363.808	212.074	17	150	123.4248
"ethyl–propyl–sulfide"	6.9338	1341.57	212.51	14	145	118.4978
"2–methyl–2–butanethiol"	6.8284	1254.885	218.759	− 3	125	99.1301
"1–pentanethiol"	6.9331	1369.479	211.314	20	153	126.6373
"hexachlorobenzene"	9.786	4597.57	355.961	114	309	309.8511
"hexafluorobenzene"	7.033	1227.98	215.5	− 3	117	80.243
"o–dichlorobenzene"	7.0703	1649.55	213.32	58	210	180.4156
"m–dichlorobenzene"	7.3037	1782.4	230.01	53	202	172.9847
"p–dichlorobenzene"	6.998	1575.11	208.52	54	204	174.0495
"m–difluorobenzene"	7.0658	1310.27	222.58	36	114	90.5067
"o–difluorobenzene"	7.0203	1310.271	222.587	31	130	93.9421
"p–difluorobenzene"	7.0881	1310.27	222.58	34	112	88.8473
"bromobenzene"	6.8606	1438.82	205.45	47	177	156.082
"chlorobenzene"	6.9781	1431.05	217.56	47	147	131.7077
"fluorobenzene"	7.187	1381.83	235.57	− 23	97	85.3241
"iodobenzene"	7.0119	1640.13	208.78	17	197	188.2415
"benzene"	6.9056	1211.033	220.79	− 16	104	80.1
"phenol"	7.1345	1516.07	174.57	72	208	181.8432
"benzenethiol"	6.9902	1529.454	203.048	52	198	169.1384
"2–picoline"	7.0324	1415.73	211.58	79	169	129.4294
"3–picoline"	7.0502	1481.77	211.21	74	185	144.1828
"aniline"	7.2418	1675.3	200.01	67	227	184.1462
"1–hexyne"	6.9121	1194.6	225	− 8	118	71.3307
"cyclohexene"	6.8724	1221.9	223.18	27	87	82.9389
"1–methylcyclopentene"	6.8688	1199.6	225	− 5	130	75.8004
"3–methylcyclopentene"	6.8726	1165.6	227	− 10	119	65.0003
"4–methylcyclopentene"	6.8702	1197.6	225	− 2	130	75.2003
"cyclohexanone"	6.9785	1495.58	209.559	90	166	155.4217
"1–hexene"	6.8657	1152.971	225.849	− 29	87	63.4855
"2–hexene,cis"	7.038	1258.571	233.851	− 25	92	68.8912
"2–hexene,trans"	6.8934	1173.343	224.53	− 25	91	67.8842
"3–hexene,cis"	6.8785	1164.134	224.749	− 27	90	66.45
"3–hexene,trans"	6.9178	1180.707	225.384	− 26	90	67.0884
"2–methyl–1–pentene"	6.8503	1138.516	224.704	− 30	85	62.113
"3–methyl–1–pentene"	6.7552	1086.316	226.204	− 37	77	54.1778
"4–methyl–1–pentene"	6.8353	1121.302	229.687	− 38	77	53.8656
"2–methyl–2–pentene"	6.9237	1183.837	225.514	− 26	90	67.3079
"3–methyl–2–pentene,cis"	6.9107	1186.402	226.696	− 26	91	67.7027
"3–methyl–2–pentene,trans"	6.9263	1194.527	224.833	− 23	94	70.4381
"4–methyl–2–pentene,cis"	6.8413	1120.707	226.586	− 35	79	56.3868
"4–methyl–2–pentene,trans"	6.8803	1142.874	227.143	− 33	81	58.6122
"2–ethyl–1–butene"	6.9971	1218.352	231.3	− 28	88	64.6819
"2,3–dimethyl–1–butene"	6.8624	1134.675	229.367	− 36	78	55.6165
"3,3–dimethyl–1–butene"	6.6775	1010.516	224.909	− 47	64	41.2477
"2,3–dimethyl–2–butene"	6.9506	1215.428	225.443	− 21	97	73.2051
"cyclohexane"	6.8413	1201.531	222.647	6	105	80.7327
"methylcyclopentane"	6.8628	1186.059	226.042	− 24	96	71.8119
"cyclohexanol"	6.2553	912.87	109.13	94	161	161.3912
"hexanal"	6.7144	1316	215.01	64	156	128.2699
"thiacycloheptane"	6.9052	1422.47	211.72	78	169	141.7399
"hexane"	6.8702	1168.72	224.21	− 25	92	68.7444
"2–methylpentane"	6.8391	1135.41	226.572	− 32	83	60.2718
"3–methylpentane"	6.8189	1152.368	227.129	− 29	89	65.4945
"2,2–dimethylbutane"	6.7548	1081.176	229.343	− 41	73	49.741
"2,3–dimethylbutane"	6.8098	1127.187	228.9	− 35	81	57.9878
"propyl–ether"	6.9476	1256.5	219	26	89	89.9663

"isopropyl–ether"	7.0971	1257.6	230.01	– 24	91	68.262
"hexyl–alcohol"	7.8604	1761.26	196.67	35	157	157.026
"butyl–ethyl–sulfide"	6.941	1421.32	205.81	33	172	144.251
"isopropyl–sulfide"	6.8712	1327.12	212.55	13	147	120.031
"methyl–pentyl–sulfide"	7.1161	1413.44	205.73	70	153	128.0003
"propyl–sulfide"	6.9358	1413.44	205.73	32	170	142.8409
"1–hexanethiol"	6.9466	1454.004	204.954	40	181	152.6619
"propyl–disulfide"	6.9753	1603.793	195.848	73	226	195.8487
"triethylamine"	6.8989	1251.8	222.01	– 13	127	89.5313
"a,a,a–trifluorotoluene"	6.9704	1306.35	217.38	55	139	102.0494
"benzonitrile"	7.7291	2110.572	244.819	28	191	190.5034
"benzoic–acid"	7.454	1820	147.96	132	287	250.012
"p–fluorotoluene"	6.9943	1374.055	217.4	68	155	116.6398
"toluene"	6.9546	1344.8	219.482	6	136	110.6253
"1,3,5–cycloheptatriene"	6.9743	1376.84	220.75	0	65	115.5965
"m–cresol"	7.508	1856.36	199.07	97	207	202.1155
"o–cresol"	6.9117	1435.5	165.16	97	207	190.9651
"p–cresol"	7.0351	1511.08	161.86	97	207	201.88
"1–heptyne"	6.6859	1216.6	220	14	142	99.7274
"1–heptene"	6.9007	1257.505	219.179	– 6	118	93.6428
"cycloheptane"	6.8539	1331.57	216.36	57	162	118.7875
"ethylcyclopentane"	6.8871	1298.599	220.675	– 3	129	103.4661
"1,1–dimethylcyclopentane"	6.8172	1219.474	221.946	– 12	113	87.8461
"c–1,2–dimethylcyclopentane"	6.8501	1269.14	220.209	– 3	125	99.5327
"t–1,2–dimethylcyclopentane"	6.8442	1242.748	221.686	– 9	117	91.8695
"c–1,3–dimethylcyclopentane"	6.8372	1237.456	222.005	– 10	116	90.7733
"t–1,3–dimethylcyclopentane"	6.8382	1240.023	221.621	– 9	117	91.7253
"methylcyclohexane"	6.823	1270.763	221.416	– 3	127	100.9338
"heptanal"	5.4759	686.453	111.817	12	155	152.7063
"heptane"	6.8938	1264.37	216.636	– 2	123	98.4297
"2–methylhexane"	6.8732	1236.026	219.545	– 9	115	90.0523
"3–methylhexane"	6.8676	1240.196	219.223	– 8	117	91.8505
"3–ethylpentane"	6.8756	1251.827	219.887	– 7	118	93.4751
"2,2–dimethylpentane"	6.8148	1190.033	223.303	– 19	104	79.1975
"2,3–dimethylpentane"	6.8538	1238.017	221.823	– 10	115	89.7841
"2,4–dimethylpentane"	6.8262	1192.041	221.634	– 17	105	80.5007
"3,3–dimethylpentane"	6.8267	1228.663	225.316	– 14	111	86.0646
"2,2,3–trimethylbutane"	6.7923	1200.563	226.05	– 19	106	80.8827
"isopropyl–tert–butyl–ether"	6.6291	1257.6	230.01	41	134	105.5006
"heptyl–alcohol"	6.6476	1140.64	126.56	60	176	176.2552
"butyl–propyl–sulfide"	6.6528	1421.32	205.81	99	203	171.0004
"ethyl–pentyl–sulfide"	6.6528	1421.32	205.81	99	203	171.0004
"hexyl–methyl–sulfide"	6.6528	1421.32	205.81	99	203	171.0004
"1–heptanethiol"	6.9525	1525.311	197.696	59	206	176.919
"ethynylbenzene"	6.957	1445.58	209.44	82	172	145.2003
"styrene"	6.9571	1445.58	209.44	32	187	145.1916
"1,3,5,7–cyclooctatetraene"	7.0067	1472.11	215.84	0	75	140.9593
"ethylbenzene"	6.9572	1424.255	213.206	26	163	136.1864
"m–xylene"	7.0091	1462.266	215.105	28	166	139.1032
"o–xylene"	6.9989	1474.679	213.686	32	172	144.4113
"p–xylene"	6.9905	1453.43	215.307	27	166	138.3509
"1–octyne"	7.0245	1413.8	215	25	170	126.1962
"1–octene"	6.9326	1353.486	212.764	15	148	121.2803
"cyclooctane"	6.8619	1437.78	209.98	94	197	151.1727
"propylcyclopentane"	6.9039	1384.386	213.159	21	158	130.9497
"ethylcyclohexane"	6.8673	1382.466	214.995	21	160	131.7948
"1,1–dimethylcyclohexane"	6.7089	1321.705	217.845	10	147	119.5427

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"1,1–dimethylcyclohexane"	6.7982	1321.705	217.845	10	147	119.5487
"c–1,2–dimethylcyclohexane"	6.8375	1367.311	215.835	18	158	129.7382
"t–1,2–dimethylcyclohexane"	6.8331	1353.881	219.132	13	151	123.4261
"c–1,3–dimethylcyclohexane"	6.8388	1338.473	218.072	11	147	120.0956
"t–1,3–dimethylcyclohexane"	6.8346	1343.687	215.394	15	152	124.4584
"c–1,4–dimethylcyclohexane"	6.8329	1345.613	216.154	15	152	124.3303
"t–1,4–dimethylcyclohexane"	6.8177	1330.437	218.581	10	147	119.3578
"octanal"	12.5117	3977.531	244.532	73	169	168.4663
"octane"	6.9094	1349.82	209.385	19	152	125.6755
"2–methylheptane"	6.9174	1337.468	213.693	12	144	117.6475
"3–methylheptane"	6.8994	1331.53	212.414	13	145	118.9256
"4–methylheptane"	6.9006	1327.661	212.568	12	144	117.7094
"3–ethylhexane"	6.891	1327.884	212.595	13	145	118.5344
"2,2–dimethylhexane"	6.8372	1273.594	215.072	3	133	106.8405
"2,3–dimethylhexane"	6.87	1315.503	214.157	10	142	115.6069
"2,4–dimethylhexane"	6.853	1287.876	214.79	5	135	109.4294
"2,5–dimethylhexane"	6.8598	1287.274	214.412	5	135	109.1028
"3,3–dimethylhexane"	6.8512	1307.882	217.439	6	138	111.9694
"3,4–dimethylhexane"	6.8799	1330.035	214.863	11	144	117.725
"3–ethyl–2–methylpentane"	6.8636	1318.12	215.306	9	142	115.6499
"3–ethyl–3–methylpentane"	6.8673	1347.209	219.684	10	145	118.2591
"2,2,3–trimethylpentane"	6.8255	1294.875	218.42	4	136	109.8414
"2,2,4–trimethylpentane"	6.8119	1257.84	220.735	−4	125	99.2384
"2,3,3–trimethylpentane"	6.8435	1328.046	220.375	7	142	114.7603
"2,3,4–trimethylpentane"	6.854	1315.084	217.526	7	140	113.4671
"2,2,3,3–tetramethylbutane"	6.8766	1329.93	226.36	103	133	106.4689
"butyl–ether"	6.9825	1431.5	207.01	32	182	141.9928
"sec–butyl–ether"	6.7915	1348.53	223.79	57	149	121.0394
"tert–butyl–ether"	6.9329	1348.533	223.79	4	109	109.0064
"octyl–alcohol"	6.837	1310.62	136.06	70	195	195.2237
"butyl–sulfide"	6.5459	1421.32	205.81	106	215	181.9909
"ethyl–hexyl–sulfide"	6.4269	1421.32	205.81	115	231	195.0003
"heptyl–methyl–sulfide"	6.4269	1421.32	205.81	115	231	195.0003
"pentyl–propyl–sulfide"	6.4269	1421.32	205.81	115	231	195.0003
"1–octanethiol"	6.9691	1593	190.61	76	229	199.0408
"butyl–disulfide"	6.9638	1684.1	181.3	101	263	231.1677
"alpha–methylstyrene"	7.0924	1582.7	206.01	75	220	169.7866
"propenylbenzene,cis"	7.4496	1909.083	238.874	18	179	178.9785
"propenylbenzene,trans"	7.5499	1909.08	238.87	105	197	170.0039
"m–methylstyrene"	6.8793	1471.44	200	72	250	168.0011
"o–methylstyrene"	6.8846	1485.41	200	75	255	171.0004
"p–methylstyrene"	7.0112	1535.1	200.7	68	170	170.9601
"propylbenzene"	6.9514	1491.297	207.14	43	188	159.2175
"cumene"	6.9367	1460.793	207.777	38	181	152.3927
"m–ethyltoluene"	7.0158	1529.184	208.509	46	190	161.3052
"o–ethyltoluene"	7.0031	1535.374	207.3	48	194	165.1533
"p–ethyltoluene"	6.998	1527.113	208.921	46	191	161.989
"1,2,3–trimethylbenzene"	7.0408	1593.958	207.078	57	205	176.0844
"1,2,4–trimethylbenzene"	7.0438	1573.267	208.564	52	198	169.3512
"mesitylene"	7.0744	1569.622	209.578	49	193	164.7167
"1–nonyne"	6.7741	1404.7	210	50	223	150.8006
"1–nonene"	6.9539	1435.359	205.535	36	174	146.8684
"butylcyclopentane"	6.8994	1457.08	205.99	41	185	156.5997
"propylcyclohexane"	6.8865	1460.8	207.939	40	186	156.7462
"c–c–135trimethylcyclohexane"	7.0974	1460.8	207.93	78	164	138.5089
"c–t–135trimethylcyclohexane"	7.0727	1460.8	207.93	80	166	140.5494
"nonanal"	7.815	2036.854	227.486	33	185	185.3142

"nonane"	6.9344	1429.46	201.82	39	179	150.8208
"2–methyloctane"	6.9119	1398.42	203.65	33	171	143.2581
"3–methyloctane"	6.9092	1405.8	204.76	33	172	144.2135
"4–methyloctane"	6.9032	1399.12	205.41	32	170	142.425
"3–ethylheptane"	6.9049	1406.5	206.5	32	171	143.0212
"4–ethylheptane"	6.899	1399.8	207.2	30	169	141.1679
"2,2–dimethylheptane"	6.8817	1363.91	208.21	24	160	132.6885
"2,3–dimethylheptane"	6.8764	1389.5	207.3	29	168	140.4631
"2,4–dimethylheptane"	6.9025	1368.72	207.44	24	160	132.8931
"2,5–dimethylheptane"	6.8932	1375.4	206.8	27	163	135.9911
"2,6–dimethylheptane"	6.8938	1368	205.68	26	162	135.209
"3,3–dimethylheptane"	6.8755	1385.36	209.79	26	165	137.0081
"3,4–dimethylheptane"	6.8836	1396.9	208.4	29	168	140.5828
"3,5–dimethylheptane"	6.9016	1382.8	207.9	26	163	136.0094
"4,4–dimethylheptane"	6.8697	1378.7	210.4	24	163	135.237
"3–ethyl–2–methylhexane"	6.8869	1390.2	209	27	166	138.022
"4–ethyl–2–methylhexane"	6.9003	1376.1	208.6	25	161	133.7572
"3–ethyl–3–methylhexane"	6.8779	1406.8	211.4	28	169	140.559
"3–ethyl–4–methylhexane"	6.8943	1404.3	209.5	29	168	140.3953
"2,2,3–trimethylhexane"	6.8657	1375.72	211.63	23	161	133.601
"2,2,4–trimethylhexane"	6.8492	1340.9	211.35	18	154	126.5438
"2,2,5–trimethylhexane"	6.8353	1324.049	210.737	16	151	124.0841
"2,3,3–trimethylhexane"	6.8542	1389.79	212.1	25	166	137.6773
"2,3,4–trimethylhexane"	6.8527	1387.22	210.22	27	167	139.0362
"2,3,5–trimethylhexane"	6.8708	1359.09	209.29	22	159	131.3369
"2,4,4–trimethylhexane"	6.8516	1368.723	214.047	20	158	130.6486
"3,3,4–trimethylhexane"	6.8576	1403.88	212.56	27	169	140.4578
"3,3–diethylpentane"	6.8926	1451.245	215.575	31	175	146.1685
"3–ethyl–2,2–dimethylpentane"	6.8717	1383.13	212.75	23	162	133.8256
"3–ethyl–2,3–dimethylpentane"	6.8446	1418	213	30	174	144.736
"3–ethyl–2,4–dimethylpentane"	6.8529	1380.54	210.87	25	165	136.6878
"2,2,3,3–tetramethylpentane"	6.8288	1397.483	213.703	26	169	140.2742
"2,2,3,4–tetramethylpentane"	6.8317	1374.042	214.762	21	161	133.016
"2,2,4,4–tetramethylpentane"	6.7971	1325.183	216.093	13	150	122.2844
"2,3,3,4–tetramethylpentane"	6.8596	1417.473	214.705	27	170	141.5517
"nonyl–alcohol"	6.6757	1276.63	123.06	90	214	213.348
"butyl–pentyl–sulfide"	6.2345	1421.32	205.81	129	258	218.0008
"ethyl–heptyl–sulfide"	6.2345	1421.32	205.81	129	258	218.0008
"hexyl–propyl–sulfide"	6.2345	1421.32	205.81	129	258	218.0008
"methyl–octyl–sulfide"	6.2345	1421.32	205.81	129	258	218.0008
"1–nonanethiol"	6.9839	1655.6	183.7	93	251	219.8011
"naphthalene"	7.0106	1733.71	201.859	87	250	217.9421
"azulene"	6.7868	1733.71	201.85	160	278	242.0097
"butylbenzene"	6.9832	1577.965	201.378	62	213	183.2704
"m–diethylbenzene"	7.0036	1575.31	200.96	61	211	181.1384
"o–diethylbenzene"	6.9878	1576.94	200.51	63	213	183.4552
"p–diethylbenzene"	6.9982	1588.31	201.97	63	214	183.7868
"1,2,3,4–tetramethylbenzene"	7.0594	1690.54	199.48	80	236	205.0922
"1,2,3,5–tetramethylbenzene"	7.0779	1675.43	201.14	75	228	198.0488
"1,2,4,5–tetramethylbenzene"	7.08	1672.43	201.43	74	227	196.8448
"1–decyne"	7.1087	1606.6	206	78	246	174.0007
"decahydronaphthalene,cis"	6.8753	1594.46	203.392	68	228	195.7742
"decahydronaphthalene,trans"	6.8568	1564.683	206.259	61	219	187.2733
"1–decene"	6.9603	1501.872	197.578	54	199	170.5706
"1–cyclopentylpentane"	6.9414	1540.6	198.8	60	210	180.6033
"butylcyclohexane"	6.9103	1538.518	200.833	59	211	180.9819
"decanal"	8.2079	2378.316	237.905	52	209	208.5488

decanal						
"decane"	6.9638	1508.75	195.374	58	203	174.1517
"2–methylnonane"	6.9337	1472.73	196.38	52	196	166.9963
"3–methylnonane"	6.9298	1479.1	197.5	52	197	167.8058
"4–methylnonane"	6.9223	1471	198.3	50	194	165.6714
"5–methylnonane"	6.9188	1468.4	198.5	50	194	165.1484
"3–ethyloctane"	6.9184	1477.4	199.4	50	195	166.5071
"4–ethyloctane"	6.9092	1466.68	200.44	48	192	163.6444
"2,2–dimethyloctane"	6.9062	1439.6	200.7	43	185	156.9329
"2,3–dimethyloctane"	6.8945	1462.22	200	48	193	164.3094
"2,4–dimethyloctane"	6.9215	1439.8	200.4	43	184	155.9291
"2,5–dimethyloctane"	6.9026	1442.5	200.2	44	187	158.4688
"2,6–dimethyloctane"	6.9333	1450.53	199.4	45	187	158.5349
"2,7–dimethyloctane"	6.9133	1444.19	198.27	46	188	159.8724
"3,3–dimethyloctane"	6.889	1457.6	202.5	45	190	161.1603
"3,4–dimethyloctane"	6.8993	1465.9	201.4	47	192	163.3927
"3,5–dimethyloctane"	6.8976	1448.8	201.3	44	188	159.3881
"3,6–dimethyloctane"	6.9128	1456.9	200.5	46	189	160.832
"4,4–dimethyloctane"	6.8889	1446.9	203.5	42	186	157.4943
"4,5–dimethyloctane"	6.8929	1460.52	201.9	46	191	162.1319
"4–propylheptane"	6.9471	1458.7	201.2	44	186	157.5303
"4–isopropylheptane"	6.8876	1449.8	202.9	43	188	158.9388
"3–ethyl–2–methylheptane"	6.8929	1457.9	202.2	45	190	161.1734
"4–ethyl–2–methylheptane"	6.892	1438.2	202.3	42	185	156.2473
"5–ethyl–2–methylheptane"	6.8942	1448.8	201.3	44	188	159.6883
"3–ethyl–3–methylheptane"	6.8806	1472.9	204.5	46	193	163.7419
"4–ethyl–3–methylheptane"	6.8869	1464.2	203.3	45	191	162.1948
"3–ethyl–5–methylheptane"	6.9159	1455.2	202.4	44	187	158.234
"3–ethyl–4–methylheptane"	6.8883	1466.8	203	46	192	163.0177
"4–ethyl–4–methylheptane"	6.883	1464.9	205.2	44	190	160.8231
"2,2,3–trimethylheptane"	6.8751	1446.1	204.4	42	187	157.6449
"2,2,4–trimethylheptane"	6.8752	1409.4	204.5	35	177	148.3408
"2,2,5–trimethylheptane"	6.8786	1417.4	203.8	37	179	150.7506
"2,2,6–trimethylheptane"	6.8945	1411.09	202.63	37	177	148.9361
"2,3,3–trimethylheptane"	6.872	1457.8	205	43	189	160.253
"2,3,4–trimethylheptane"	6.8742	1451.7	203.6	44	189	159.9288
"2,3,5–trimethylheptane"	6.8399	1440	203	44	190	160.7203
"2,3,6–trimethylheptane"	6.8867	1433.7	201.9	42	184	156.0001
"2,4,4–trimethylheptane"	6.8606	1418.4	205.4	37	180	150.9992
"2,4,5–trimethylheptane"	6.8758	1437.3	203.3	41	185	156.4732
"2,4,6–trimethylheptane"	6.914	1411.3	202.3	36	175	147.6262
"2,5,5–trimethylheptane"	6.882	1429.09	204.36	39	181	152.803
"3,3,4–trimethylheptane"	6.8686	1466.8	205.9	44	191	161.9222
"3,3,5–trimethylheptane"	6.8552	1435.43	205.49	40	185	155.6766
"3,4,4–trimethylheptane"	6.8672	1464.1	206.2	43	190	161.0741
"3,4,5–trimethylheptane"	6.8711	1463.4	204.2	45	192	162.5378
"3–isopropyl–2–methylhexane"	6.761	1441	204.7	45	197	166.671
"3,3–diethylhexane"	6.8836	1490.9	206.2	47	196	166.2702
"3,4–diethylhexane"	6.8835	1473.2	204.2	46	193	163.8556
"3–ethyl–2,2–dimethylhexane"	6.8659	1444.4	206.4	40	185	156.0477
"4–ethyl–2,2–dimethylhexane"	6.8953	1416	206	34	175	146.7261
"3–ethyl–2,3–dimethylhexane"	6.8613	1475.8	206.8	45	194	163.9606
"4–ethyl–2,3–dimethylhexane"	6.8682	1458	204.7	44	190	160.9503
"3–ethyl–2,4–dimethylhexane"	6.8668	1455.3	205	43	189	160.1023
"4–ethyl–2,4–dimethylhexane"	6.8672	1464.1	206.2	43	190	161.0741
"3–ethyl–2,5–dimethylhexane"	6.8716	1429.3	204.1	39	183	154.0544
"4–ethyl–3,3–dimethylhexane"	6.8629	1473.1	207	44	193	162.9336

"3–ethyl–3,4–dimethylhexane"	6.8615	1470.4	207.3	44	192	162.0854
"2,2,3,3–tetramethylhexane"	6.8444	1464.03	209.06	41	190	160.3119
"2,2,3,4–tetramethylhexane"	6.8241	1443.6	207.3	41	188	158.7906
"2,2,3,5–tetramethylhexane"	6.8768	1417.6	206.3	35	177	148.4515
"2,2,4,4–tetramethylhexane"	6.7315	1396	208.7	35	184	153.8318
"2,2,4,5–tetramethylhexane"	6.8356	1400.55	206.26	34	176	147.8796
"2,2,5,5–tetramethylhexane"	6.8812	1377.98	207	27	165	137.4583
"2,3,3,4–tetramethylhexane"	6.8424	1474.94	207.72	45	195	164.5876
"2,3,3,5–tetramethylhexane"	6.8504	1429.2	206.9	37	182	153.1348
"2,3,4,4–tetramethylhexane"	6.8294	1457.9	207.6	42	191	161.6207
"2,3,4,5–tetramethylhexane"	6.8716	1442.8	205.3	40	185	156.2364
"3,3,4,4–tetramethylhexane"	6.8116	1492.7	209.7	47	201	170.042
"24dimethyl3isopropylpentane"	6.8215	1432.15	206.38	40	186	157.0428
"3,3–diethyl–2–methylpentane"	6.8598	1501.8	207.7	49	200	169.729
"3–ethyl–2,2,3–trimethylpentane"	6.8071	1490.1	210	47	200	169.5189
"3–ethyl–2,2,4–trimethylpentane"	6.8315	1435.6	208.1	38	185	155.2808
"3–ethyl–2,3,4–trimethylpentane"	6.8162	1486.62	208.32	47	200	169.4409
"2,2,3,3,4–pentamethylpentane"	6.7966	1474.89	210.6	44	197	166.0533
"2,2,3,4,4–pentamethylpentane"	6.7327	1423.83	210.35	38	190	159.292
"decyl–alcohol"	6.9224	1472.01	134.16	103	230	230.0559
"butyl–hexyl–sulfide"	6.069	1421.32	205.81	143	285	240.0011
"ethyl–octyl–sulfide"	6.069	1421.32	205.81	143	285	240.0011
"heptyl–propyl–sulfide"	6.069	1421.32	205.81	143	285	240.0011
"methyl–nonyl–sulfide"	6.069	1421.32	205.81	143	285	240.0011
"pentyl–sulfide"	6.069	1421.32	205.81	143	285	240.0011
"1–decanethiol"	6.9981	1713.6	177	109	271	239.1965
"pentyl–disulfide"	6.9581	1756	166.8	128	298	263.8786
"1–methylnaphthalene"	7.0359	1826.948	195.002	108	278	244.6854
"2–methylnaphthalene"	7.0685	1840.268	198.395	105	274	241.0524
"pentylbenzene"	6.9783	1639.91	194.76	80	237	205.4605
"pentamethylbenzene"	7.1376	1833.8	198.96	125	270	231.8345
"1–undecyne"	7.1306	1687.2	202	80	267	195.0045
"1–undecene"	6.9666	1562.469	189.743	72	222	192.6709
"1–cyclopentylhexane"	6.9548	1608	191.6	78	234	203.0994
"pentylcyclohexane"	6.9467	1619.11	194.51	78	235	203.7111
"undecane"	6.9722	1569.57	187.7	75	226	195.9279
"undecyl–alcohol"	6.5271	1250	100	120	243	242.8145
"butyl–heptyl–sulfide"	5.9321	1421.32	205.81	155	309	260.0001
"decyl–methyl–sulfide"	5.9321	1421.32	205.81	155	309	260.0001
"ethyl–nonyl–sulfide"	5.9321	1421.32	205.81	155	309	260.0001
"octyl–propyl–sulfide"	5.9321	1421.32	205.81	155	309	260.0001
"1–undecanethiol"	7.0122	1767.4	170.4	124	290	257.3983
"biphenyl"	7.2454	1998.72	202.74	70	272	255.2003
"1–ethylnaphthalene"	7.0316	1841.32	185.28	120	292	258.3286
"2–ethylnaphthalene"	7.0757	1880.73	191.41	118	291	256.933
"1,2–dimethylnaphthalene"	7.006	1805.31	171.37	129	269	266.2558
"1,3–dimethylnaphthalene"	7.2698	2076	210	148	310	263.0021
"1,4–dimethylnaphthalene"	7.2698	2076	210	148	310	263.0021
"1,5–dimethylnaphthalene"	7.0493	1855	180	150	313	265.0056
"1,6–dimethylnaphthalene"	7.2698	2076	210	148	310	263.0021
"1,7–dimethylnaphthalene"	7.0564	1879	180	150	320	269.9967
"2,3–dimethylnaphthalene"	7.0527	1869	180	155	315	267.9988
"2,6–dimethylnaphthalene"	7.046	1841	180	150	310	261.997
"2,7–dimethylnaphthalene"	7.0478	1846	180	150	310	263.006
"hexylbenzene"	6.9853	1700.5	188.2	96	258	226.1027
"1,2,3–triethylbenzene"	7.5888	2133.55	235.68	146	247	217.4996
"1,2,4–triethylbenzene"	7.5787	2133.558	235.681	46	218	218.4727

"1,3,5–triethylbenzene"	7.6044	2133.55	235.68	145	246	216.0001
"hexamethylbenzene"	7.1554	2133.55	235.68	178	300	263.4396
"1–dodecyne"	7.1693	1771.1	198	113	288	214.9905
"1–dodecene"	6.9752	1619.862	182.271	89	244	213.357
"1–cyclopentylheptane"	6.9743	1672.2	184.4	95	256	224.1026
"1–cyclohexylhexane"	6.9555	1681	187.8	94	257	224.7471
"dodecane"	6.998	1639.27	181.835	91	247	216.3228
"dodecyl–alcohol"	7.5399	2003.29	168.13	138	214	261.8485
"butyl–octyl–sulfide"	6.629	1408	116.06	134	307	259.5883
"decyl–ethyl–sulfide"	5.8125	1421.32	205.81	166	333	279.0015
"hexyl–sulfide"	5.8125	1421.32	205.81	166	333	279.0015
"methyl–undecyl–sulfide"	5.8125	1421.32	205.81	166	333	279.0015
"nonyl–propyl–sulfide"	5.8125	1421.32	205.81	166	333	279.0015
"1–dodecanethiol"	7.0244	1817.8	164.1	138	308	274.6021
"hexyl–disulfide"	6.9632	1824.9	153.5	153	328	293.5179
"1–propylnaphthalene"	7.0594	1890.8	180	155	335	272.4975
"2–propylnaphthalene"	7.0605	1895.5	180	160	335	273.5029
"2–ethyl–3–methylnaphthalene"	7.0285	1895.5	180	196	312	277.0007
"2–ethyl–6–methylnaphthalene"	7.093	1895.5	180	192	303	270.0006
"2–ethyl–7–methylnaphthalene"	7.093	1895.5	180	192	303	270.0006
"1–phenylheptane"	7.0006	1761.2	181.5	112	279	245.9979
"1–tridecyne"	7.1567	1834.4	195	120	308	234.0064
"1–tridecene"	6.9856	1674.741	175.214	105	264	232.7801
"1–cyclopentyloctane"	6.9896	1729.8	177.3	112	276	243.7002
"1–cyclohexylheptane"	6.9743	1743	180.9	111	278	244.8984
"tridecane"	7.0076	1690.67	174.22	107	267	235.4659
"1–tridecanol"	7.4118	2003.29	168.13	202	304	274.0001
"butyl–nonyl–sulfide"	5.7076	1421.32	205.81	177	355	297.0013
"decyl–propyl–sulfide"	5.7076	1421.32	205.81	177	355	297.0013
"dodecyl–methyl–sulfide"	5.7076	1421.32	205.81	177	355	297.0013
"ethyl–undecyl–sulfide"	5.7076	1421.32	205.81	177	355	297.0013
"1–tridecanethiol"	7.037	1864.9	157.9	151	325	290.8046
"1–butylnaphthalene"	4.9631	656.8	26	139	292	289.4225
"2–butylnaphthalene"	6.6117	1591.4	138.5	145	291	288.0474
"1–phenyloctane"	7.0086	1812.2	174.6	127	298	264.4247
"1,2,3,4–tetraethylbenzene"	7.6563	2312.864	236.261	66	248	248.0571
"1,2,3,5–tetraethylbenzene"	7.6324	2312.86	236.26	174	282	250.5004
"1,2,4,5–tetraethylbenzene"	7.6372	2312.86	236.26	174	282	250.001
"1–tetradecyne"	7.2323	1927.7	191	145	326	252.0011
"1–tetradecene"	7.02	1745.001	170.475	119	283	251.1006
"1–cyclopentylnonane"	6.996	1779	170.2	126	296	262.1012
"1–cyclohexyloctane"	6.9897	1799.3	174.3	126	298	263.6045
"tetradecane"	7.013	1740.88	167.72	122	286	253.5775
"1–tetradecanol"	6.6741	1204.5	54	130	264	263.5347
"butyl–decyl–sulfide"	5.6151	1421.32	205.81	187	376	314.0001
"dodecyl–ethyl–sulfide"	5.6151	1421.32	205.81	187	376	314.0001
"heptyl–sulfide"	5.6151	1421.32	205.81	187	376	314.0001
"methyl–tridecyl–sulfide"	5.6151	1421.32	205.81	187	376	314.0001
"propyl–undecyl–sulfide"	5.6151	1421.32	205.81	187	376	314.0001
"1–tetradecanethiol"	7.0485	1909.2	151.9	164	341	306.1959
"heptyl–disulfide"	6.9602	1878.6	139.8	175	357	320.7104
"1–pentylnaphthalene"	7.0743	2000	170	185	360	306.9301
"2–pentylnaphthalene"	7.06	2005.9	170	190	370	309.9738
"1–phenylnonane"	7.0245	1862.6	167.5	142	316	282.0031
"1–pentadecyne"	7.2055	1972.07	188	140	349	267.9998
"1–pentadecene"	7.0156	1781.974	162.582	134	302	268.3944

"1–cyclopentyldecane"	7.0035	1825.748	163.479	141	314	279.376
"1–cyclohexylnonane"	7.0006	1850.2	167.6	141	316	281.501
"pentadecane"	7.0236	1789.95	161.38	136	304	270.6853
"1–pentadecanol"	6.2374	1204.5	54	230	339	304.8499
"butyl–undecyl–sulfide"	5.5335	1421.32	205.81	196	397	330.0001
"dodecyl–propyl–sulfide"	5.5335	1421.32	205.81	196	397	330.0001
"ethyl–tridecyl–sulfide"	5.5335	1421.32	205.81	196	397	330.0001
"methyl–tetradecyl–sulfide"	5.5335	1421.32	205.81	196	397	330.0001
"1–pentadecanethiol"	7.0612	1951	146	176	356	320.7033
"1–phenyldecane"	7.0364	1904.132	160.318	155	333	297.89
"pentaethylbenzene"	8.295	2972.77	272.052	86	277	277.0236
"1–hexadecyne"	7.4751	2154.7	185	172	367	283.9946
"1–hexadecene"	7.0444	1843.581	157.917	147	319	284.873
"1–cyclopentylundecane"	7.02	1869.2	156	154	330	295.5863
"1–cyclohexyldecane"	7.0185	1899.242	161.348	154	333	297.6604
"hexadecane"	7.0287	1830.51	154.45	149	321	286.8647
"1–hexadecanol"	6.1586	1380	91	145	190	330.0158
"butyl–dodecyl–sulfide"	5.4612	1421.32	205.81	204	416	345.0003
"ethyl–tetradecyl–sulfide"	5.4612	1421.32	205.81	204	416	345.0003
"methyl–pentadecyl–sulfide"	5.4612	1421.32	205.81	204	416	345.0003
"octyl–sulfide"	5.4612	1421.32	205.81	204	416	345.0003
"propyl–tridecyl–sulfide"	5.4612	1421.32	205.81	204	416	345.0003
"1–hexadecanethiol"	7.075	1990	140	188	370	334.4663
"octyl–disulfide"	6.9579	1935.6	129	196	383	345.7508
"1–phenylundecane"	7.0509	1944.1	153	168	349	313.2014
"1–heptadecyne"	7.4883	2216.2	182	184	384	299.0008
"1–heptadecene"	7.0392	1877.91	151.53	159	335	300.0604
"1–cyclopentyldodecane"	7.0319	1909.1	149	168	346	310.9037
"1–cyclohexylundecane"	7.029	1939.7	154.5	167	349	313.1019
"heptadecane"	7.0143	1865.1	149.2	161	337	302.0172
"1–heptadecanol"	6.782	1595	85.06	191	383	323.79
"butyl–tridecyl–sulfide"	5.3973	1421.32	205.81	212	434	359.0001
"ethyl–pentadecyl–sulfide"	5.3973	1421.32	205.81	212	434	359.0001
"hexadecyl–methyl–sulfide"	5.3973	1421.32	205.81	212	434	359.0001
"propyl–tetradecyl–sulfide"	5.3973	1421.32	205.81	212	434	359.0001
"1–heptadecanethiol"	7.081	2027	135	198	384	347.5976
"1–phenyldodecane"	7.0693	1981.6	145.5	181	363	327.6065
"hexaethylbenzene"	7.5029	2360.733	212.652	134	298	298.1007
"1–octadecyne"	7.5079	2281.1	180	196	400	312.9916
"1–octadecene"	7.0452	1917.9	145.9	171	350	314.6503
"1–cycopentyltridecane"	7.0473	1947	141.9	180	361	325.4002
"1–cyclohexyldodecane"	7.0362	1976.7	148	179	364	327.6958
"octadecane"	7.0022	1894.3	143.3	172	352	316.3269
"1–octadecanol"	6.814	1632	80.06	201	385	334.8708
"butyl–tetradecyl–sulfide"	5.3364	1421.32	205.81	220	452	373.0008
"ethyl–hexadecyl–sulfide"	5.3364	1421.32	205.81	220	452	373.0008
"heptadecyl–methyl–sulfide"	5.3364	1421.32	205.81	220	452	373.0008
"nonyl–sulfide"	5.3364	1421.32	205.81	220	452	373.0008
"pentadecyl–propyl–sulfide"	5.3364	1421.32	205.81	220	452	373.0008
"1–octadecanethiol"	7.096	2061	129	209	397	359.9463
"nonyl–disulfide"	6.9605	1981.5	117	215	407	368.6991
"1–phenyltridecane"	7.0843	2013.9	137.9	193	377	341.2023
"1–nonadecyne"	7.5171	2336.7	177	208	416	327.0014
"1–nonadecene"	7.0571	1961.6	141.2	183	364	328.4996
"1–cyclopentyltetradecane"	7.063	1982	135	192	375	338.9148
"1–cyclohexyltridecane"	7.0469	2012.2	141.5	191	378	341.4953
"nonadecane"	7.0153	1932.8	137.6	184	366	329.8825

"1−nonadecanol"	6.6077	1632	80.06	274	395	357.8402
"butyl−pentadecyl−sulfide"	5.2825	1421.32	205.81	227	468	386.0007
"ethyl−heptadecyl−sulfide"	5.2825	1421.32	205.81	227	468	386.0007
"hexadecyl−propyl−sulfide"	5.2825	1421.32	205.81	227	468	386.0007
"methyl−octadecyl−sulfide"	5.2825	1421.32	205.81	227	468	386.0007
"1−nonadecanethiol"	7.105	2094	124	219	409	371.7168
"1−phenyltetradecane"	7.101	2042	130	205	390	353.8649
"1−eicosyne"	7.5234	2386.3	174	219	431	340.0067
"1−eicosene"	7.0577	1995.3	136	193	378	341.7003
"1−cyclopentylpentadecane"	7.083	2016	128	203	388	351.7503
"1−cyclohexyltetradecane"	7.061	2046	135	203	392	354.4519
"eicosane"	7.1522	2032.7	132.1	198	379	343.7876
"1−eicosanol"	6.872	1699	70.06	219	406	355.628
"butyl−hexadecyl−sulfide"	5.2347	1421.32	205.81	233	484	398.0007
"decyl−sulfide"	5.2347	1421.32	205.81	233	484	398.0007
"ethyl−octadecyl−sulfide"	5.2347	1421.32	205.81	233	484	398.0007
"heptadecyl−propyl−sulfide"	5.2347	1421.32	205.81	233	484	398.0007
"methyl−nonadecyl−sulfide"	5.2347	1421.32	205.81	233	484	398.0007
"1−eicosanethiol"	7.114	2125	119	229	421	382.9859
"decyl−disulfide"	6.972	2019	103.1	235	429	390.3999
"1−phenylpentadecane"	7.114	2067	122	216	403	366.2847
"1−cyclopentylhexadecane"	7.103	2048	121	215	401	364.0567
"1−cyclohexylpentadecane"	7.072	2078	129	213	404	366.8023
"1−phenylhexadecane"	7.14	2095	114	227	415	377.878
"1−cyclohexylhexadecane"	7.074	2099	122	224	416	378.574

$\text{Comp}_1 := \text{Antoine}$ $\text{Comp}_2 := \text{Antoine}$

Este programa cuenta con una base de 700 compuestos.

Selecciona los componentes de la mezcla binaria, sin importar el orden.
El programa los ordena del más volátil al menos volátil

Selecciona el compuesto 1 del sistema

toluene

$Comp_1$

Selecciona el compuesto 2 del sistema

benzene

$a := Comp_1 \qquad b := Comp_2$

if $Comp_{1_{17}} \le Comp_{2_{17}}$
  $Comp_1 := a$
  $Comp_2 := b$
else
  $Comp_1 := b$
  $Comp_2 := a$

$Tabla_1 := [\text{"Componente"}\ \text{"A"}\ \text{"B"}\ \text{"C"}\ \text{"Tb °C"}]$

$$CA := \begin{bmatrix} Comp_{1_{11}} & Comp_{1_{12}} & Comp_{1_{13}} & Comp_{1_{14}} & Comp_{1_{17}} \\ Comp_{2_{11}} & Comp_{2_{12}} & Comp_{2_{13}} & Comp_{2_{14}} & Comp_{2_{17}} \end{bmatrix}$$

$Tabla2 := [\text{"Componente"}\ \text{"T min °C"}\ \text{"T Max °C"}\ \text{"T b °C"}]$

$$TABLE2 := \begin{bmatrix} Comp_{1_{11}} & Comp_{1_{15}} & Comp_{1_{16}} & Comp_{1_{17}} \\ Comp_{2_{11}} & Comp_{2_{15}} & Comp_{2_{16}} & Comp_{2_{17}} \end{bmatrix}$$

Constantes de Antoine				
Componente	A	B	C	Tb °C
benzene	6.906	1211.033	220.790	80.100
toluene	6.955	1344.800	219.482	110.625

* Las constantes de Antoine se encuentran en mmHg y °C

* Tb = Temperatura de Ebullición @ 1 Atm

Estos coeficientes de Antoine solo deben usarse dentro del rango de temperatura indicado (T min y T Max)

Rango de Temperaturas			
Componente	T min °C	T Max °C	T b °C
benzene	-16.000	104.000	80.100
toluene	6.000	136.000	110.625

Equilibrio Líquido Vapor

Ingresa la presión del sistema en mmHg

$P := 760$

$$A := \begin{bmatrix} Comp_{1,12} \\ Comp_{2,12} \end{bmatrix} \qquad B := \begin{bmatrix} Comp_{1,13} \\ Comp_{2,13} \end{bmatrix} \qquad C := \begin{bmatrix} Comp_{1,14} \\ Comp_{2,14} \end{bmatrix}$$

$$T_K := \overrightarrow{\frac{B}{A - \log10(P)} - C} \qquad Temp := T_K \ °C$$

Temperaturas (Rango de 11 Valores)

$$T_1 := T_{K_2} \qquad T_2 := T_{K_2} - \frac{T_{K_2} - T_{K_1}}{10} \qquad T_3 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 2\right) \qquad T_4 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 3\right)$$

$$T_5 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 4\right) \qquad T_6 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 5\right) \qquad T_7 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 6\right)$$

$$T_8 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 7\right) \qquad T_9 := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 8\right) \qquad T_{10} := T_{K_2} - \left(\frac{T_{K_2} - T_{K_1}}{10} \cdot 9\right) \qquad T_{11} := T_{K_1}$$

Presiones del componentemas más volátil (Rango de 11 Valores)

$$P^{\circ}_{1.1} := 10^{\left(A_1 - \frac{B_1}{T_1 + C_1}\right)} \qquad P^{\circ}_{1.2} := 10^{\left(A_1 - \frac{B_1}{T_2 + C_1}\right)} \qquad P^{\circ}_{1.3} := 10^{\left(A_1 - \frac{B_1}{T_3 + C_1}\right)} \qquad P^{\circ}_{1.4} := 10^{\left(A_1 - \frac{B_1}{T_4 + C_1}\right)}$$

$$P^{\circ}_{1.5} := 10^{\left(A_1 - \frac{B_1}{T_5 + C_1}\right)} \qquad P^{\circ}_{1.6} := 10^{\left(A_1 - \frac{B_1}{T_6 + C_1}\right)} \qquad P^{\circ}_{1.7} := 10^{\left(A_1 - \frac{B_1}{T_7 + C_1}\right)} \qquad P^{\circ}_{1.8} := 10^{\left(A_1 - \frac{B_1}{T_8 + C_1}\right)}$$

$$P^{\circ}_{1.9} := 10^{\left(A_1 - \frac{B_1}{T_9 + C_1}\right)} \qquad P^{\circ}_{1.10} := 10^{\left(A_1 - \frac{B_1}{T_{10} + C_1}\right)} \qquad P^{\circ}_{1.11} := 10^{\left(A_1 - \frac{B_1}{T_{11} + C_1}\right)}$$

Presiones del componentemas menos volátil (Rango de 11 Valores)

$$P^{\circ}_{2.1} := 10^{\left(A_2 - \frac{B_2}{T_1 + C_2}\right)} \quad P^{\circ}_{2.2} := 10^{\left(A_2 - \frac{B_2}{T_2 + C_2}\right)} \quad P^{\circ}_{2.3} := 10^{\left(A_2 - \frac{B_2}{T_3 + C_2}\right)} \quad P^{\circ}_{2.4} := 10^{\left(A_2 - \frac{B_2}{T_4 + C_2}\right)}$$

$$P^{\circ}_{2.5} := 10^{\left(A_2 - \frac{B_2}{T_5 + C_2}\right)} \quad P^{\circ}_{2.6} := 10^{\left(A_2 - \frac{B_2}{T_6 + C_2}\right)} \quad P^{\circ}_{2.7} := 10^{\left(A_2 - \frac{B_2}{T_7 + C_2}\right)} \quad P^{\circ}_{2.8} := 10^{\left(A_2 - \frac{B_2}{T_8 + C_2}\right)}$$

$$P^{\circ}_{2.9} := 10^{\left(A_2 - \frac{B_2}{T_9 + C_2}\right)} \quad P^{\circ}_{2.10} := 10^{\left(A_2 - \frac{B_2}{T_{10} + C_2}\right)} \quad P^{\circ}_{2.11} := 10^{\left(A_2 - \frac{B_2}{T_{11} + C_2}\right)}$$

Composición en la fase líquida del componente más volátil

$$X_1 := \frac{\overrightarrow{P - P^{\circ}_{2.1}}}{P^{\circ}_{1.1} - P^{\circ}_{2.1}} \quad X_2 := \frac{\overrightarrow{P - P^{\circ}_{2.2}}}{P^{\circ}_{1.2} - P^{\circ}_{2.2}} \quad X_3 := \frac{\overrightarrow{P - P^{\circ}_{2.3}}}{P^{\circ}_{1.3} - P^{\circ}_{2.3}} \quad X_4 := \frac{\overrightarrow{P - P^{\circ}_{2.4}}}{P^{\circ}_{1.4} - P^{\circ}_{2.4}} \quad X_5 := \frac{\overrightarrow{P - P^{\circ}_{2.5}}}{P^{\circ}_{1.5} - P^{\circ}_{2.5}}$$

$$X_6 := \frac{\overrightarrow{P - P^{\circ}_{2.6}}}{P^{\circ}_{1.6} - P^{\circ}_{2.6}} \quad X_7 := \frac{\overrightarrow{P - P^{\circ}_{2.7}}}{P^{\circ}_{1.7} - P^{\circ}_{2.7}} \quad X_8 := \frac{\overrightarrow{P - P^{\circ}_{2.8}}}{P^{\circ}_{1.8} - P^{\circ}_{2.8}} \quad X_9 := \frac{\overrightarrow{P - P^{\circ}_{2.9}}}{P^{\circ}_{1.9} - P^{\circ}_{2.9}} \quad X_{10} := \frac{\overrightarrow{P - P^{\circ}_{2.10}}}{P^{\circ}_{1.10} - P^{\circ}_{2.10}}$$

$$X_{11} := \frac{\overrightarrow{P - P^{\circ}_{2.11}}}{P^{\circ}_{1.11} - P^{\circ}_{2.11}}$$

Composición en la fase vaor del componente más volátil

$$Y_1 := \frac{\overrightarrow{X_1 \cdot P^{\circ}_{1.1}}}{P} \quad Y_2 := \frac{\overrightarrow{X_2 \cdot P^{\circ}_{1.2}}}{P} \quad Y_3 := \frac{\overrightarrow{X_3 \cdot P^{\circ}_{1.3}}}{P} \quad Y_4 := \frac{\overrightarrow{X_4 \cdot P^{\circ}_{1.4}}}{P} \quad Y_5 := \frac{\overrightarrow{X_5 \cdot P^{\circ}_{1.5}}}{P} \quad Y_6 := \frac{\overrightarrow{X_6 \cdot P^{\circ}_{1.6}}}{P}$$

$$Y_7 := \frac{\overrightarrow{X_7 \cdot P^{\circ}_{1.7}}}{P} \quad Y_8 := \frac{\overrightarrow{X_8 \cdot P^{\circ}_{1.8}}}{P} \quad Y_9 := \frac{\overrightarrow{X_9 \cdot P^{\circ}_{1.9}}}{P} \quad Y_{10} := \frac{\overrightarrow{X_{10} \cdot P^{\circ}_{1.10}}}{P} \quad Y_{11} := \frac{\overrightarrow{X_{11} \cdot P^{\circ}_{1.11}}}{P}$$

$$RSB := \begin{bmatrix} \text{"Temperatra °C"} & \text{"P°1 mmHg"} & \text{"P°2 mmHg"} & \text{"X"} & \text{"Y"} \\ T_1 & P°_{1.1} & P°_{2.1} & X_1 & Y_1 \\ T_2 & P°_{1.2} & P°_{2.2} & X_2 & Y_2 \\ T_3 & P°_{1.3} & P°_{2.3} & X_3 & Y_3 \\ T_4 & P°_{1.4} & P°_{2.4} & X_4 & Y_4 \\ T_5 & P°_{1.5} & P°_{2.5} & X_5 & Y_5 \\ T_6 & P°_{1.6} & P°_{2.6} & X_6 & Y_6 \\ T_7 & P°_{1.7} & P°_{2.7} & X_7 & Y_7 \\ T_8 & P°_{1.8} & P°_{2.8} & X_8 & Y_8 \\ T_9 & P°_{1.9} & P°_{2.9} & X_9 & Y_9 \\ T_{10} & P°_{1.10} & P°_{2.10} & X_{10} & Y_{10} \\ T_{11} & P°_{1.11} & P°_{2.11} & X_{11} & Y_{11} \end{bmatrix}$$

$$X := \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ X_9 \\ X_{10} \\ X_{11} \end{bmatrix} \quad Y := \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \\ Y_6 \\ Y_7 \\ Y_8 \\ Y_9 \\ Y_{10} \\ Y_{11} \end{bmatrix} \quad Temperatura := \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \\ T_{10} \\ T_{11} \end{bmatrix} \quad P°_1 := \begin{bmatrix} P°_{1.1} \\ P°_{1.2} \\ P°_{1.3} \\ P°_{1.4} \\ P°_{1.5} \\ P°_{1.6} \\ P°_{1.7} \\ P°_{1.8} \\ P°_{1.9} \\ P°_{1.10} \\ P°_{1.11} \end{bmatrix} \quad P°_2 := \begin{bmatrix} P°_{2.1} \\ P°_{2.2} \\ P°_{2.3} \\ P°_{2.4} \\ P°_{2.5} \\ P°_{2.6} \\ P°_{2.7} \\ P°_{2.8} \\ P°_{2.9} \\ P°_{2.10} \\ P°_{2.11} \end{bmatrix}$$

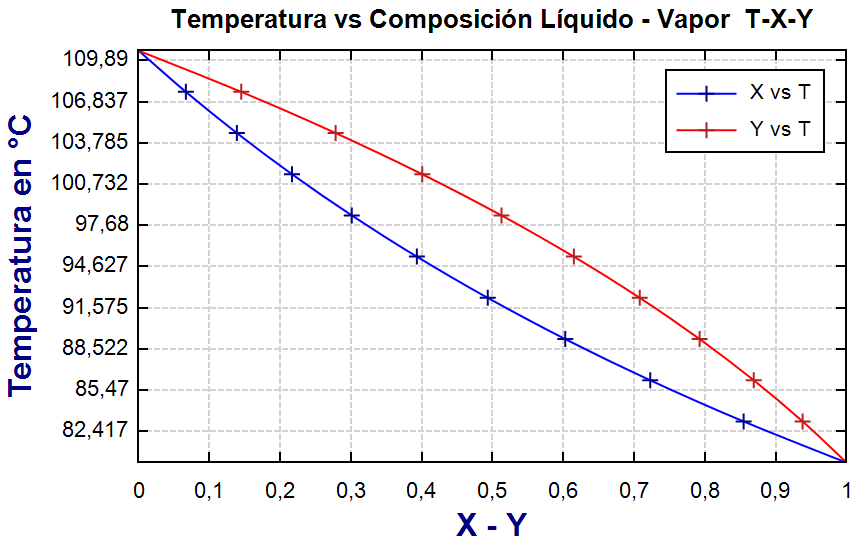
Temperatura de Saturación 1 en °C

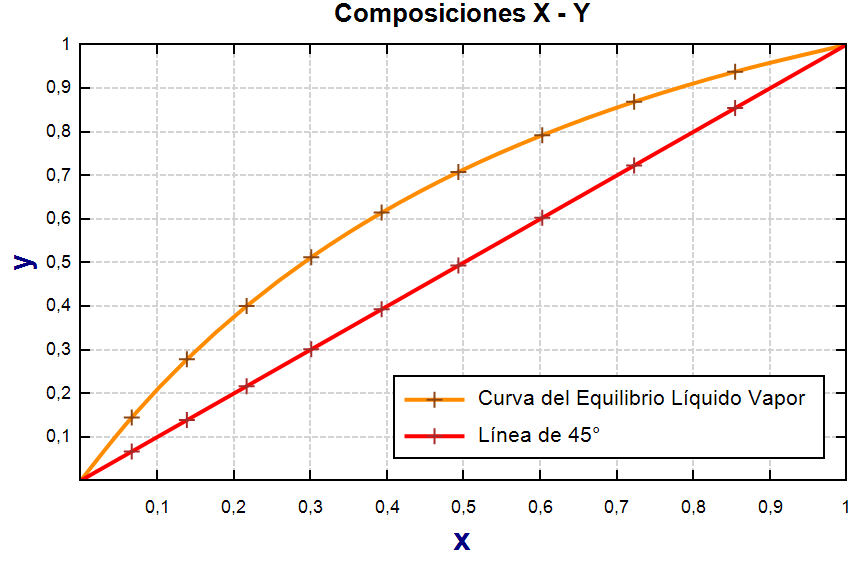
$Temp_1 = 80.1037\ °C$

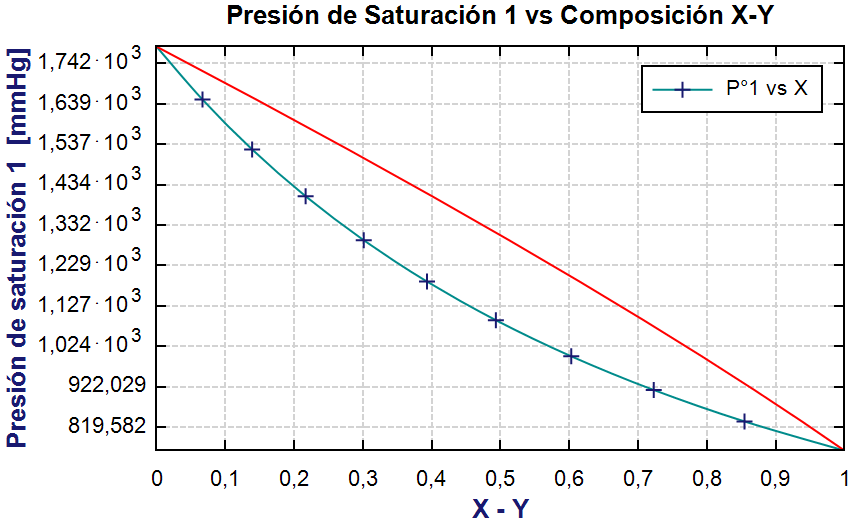
Temperatura de Saturación 2 en °C

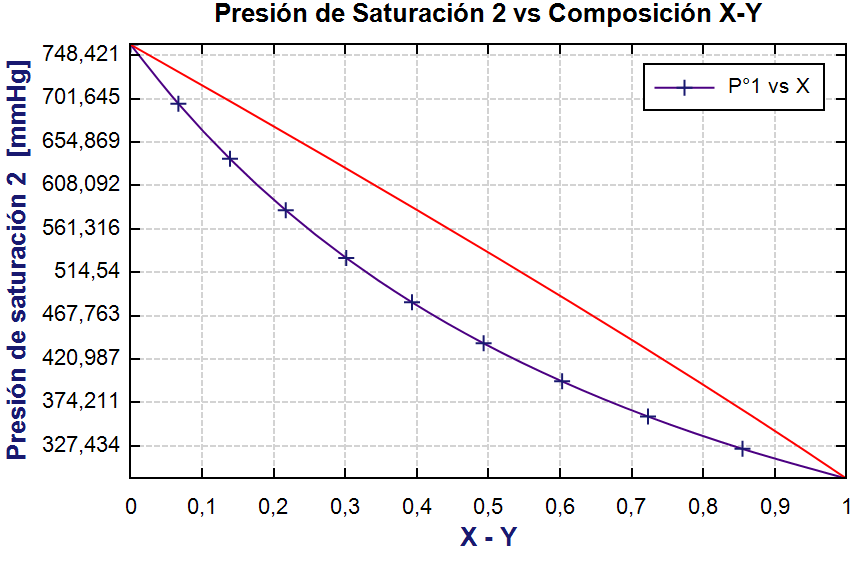
$Temp_2 = 110.6286\ °C$

Equilibrio Líquido Vapor				
Temperatra °C	P°1 mmHg	P°2 mmHg	X	Y
110.629	1784.477	760.000	0.000	0.000
107.576	1650.223	696.293	0.067	0.145
104.524	1523.831	636.876	0.139	0.278
101.471	1404.997	581.541	0.217	0.401
98.419	1293.420	530.087	0.301	0.513
95.366	1188.803	482.319	0.393	0.615
92.314	1090.853	438.045	0.493	0.708
89.261	999.279	397.078	0.603	0.792
86.209	913.798	359.238	0.723	0.869
83.156	834.130	324.347	0.855	0.938
80.104	760.000	292.237	1.000	1.000

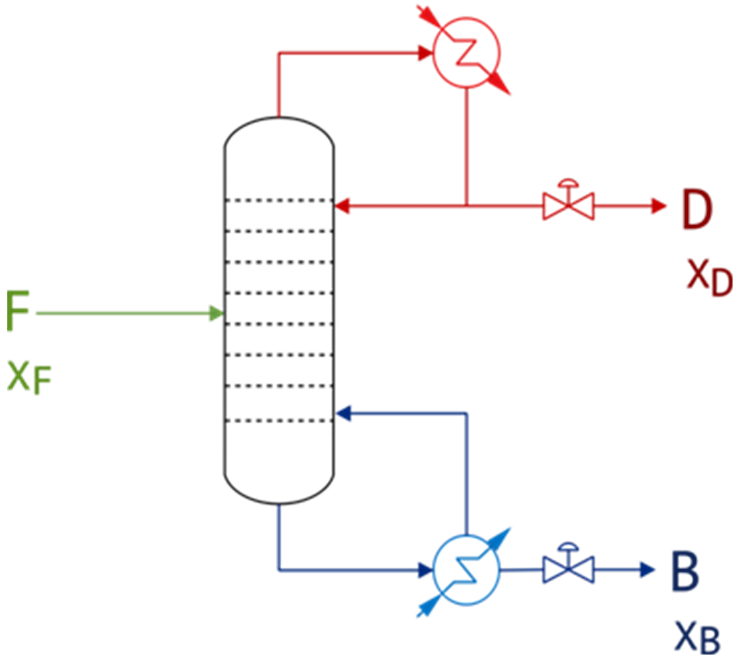

Temperatura vs Composición Líquido - Vapor T-X-Y
Temperatura en °C
109,89
106,837
103,785
100,732
97,68
94,627
91,575
88,522
85,47
82,417
0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1
X - Y
X vs T
Y vs T


Composiciones X - Y
y
1
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1
x
Curva del Equilibrio Líquido Vapor
Línea de 45°


Presión de Saturación 1 vs Composición X-Y
Presión de saturación 1 [mmHg]
1,742·10^3
1,639·10^3
1,537·10^3
1,434·10^3
1,332·10^3
1,229·10^3
1,127·10^3
1,024·10^3
922,029
819,582
P°1 vs X
0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1
X - Y


Presión de Saturación 2 vs Composición X-Y
Presión de saturación 2 [mmHg]
748,421
701,645
654,869
608,092
561,316
514,54
467,763
420,987
374,211
327,434
P°1 vs X
0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1
X - Y

Mc Cabe – Thiele



Flujo molar que ingresa a la columna "F"

$F := 350 \ \frac{kmol}{hr}$

Composición del Destilado "XD"

$x_D := 97 \ \%$

Composición en los Fondos "XB"

$x_B := 2 \ \%$

Composición de la Alimentación "XF"

$z := 40 \ \%$

Calidad de la alimentación "q"

$q := 1.5$

Relación de Reflujo "R"

$R := 3.5$

Balance de materia para D y B

$$F = D + B \qquad F \cdot z = D \cdot x_D + B \cdot x_B$$

Flujo Molar del Destilado

$$D = 140\ \frac{\text{kmol}}{\text{hr}}$$

Flujo Molar en los Fondos

$$B = 210\ \frac{\text{kmol}}{\text{hr}}$$

Balance de materia para la zona de Rectificación "Condensador"

$$R = \frac{L}{D} \qquad L_D := R \cdot D \qquad V_D := D + L_D \qquad V_B := V_D$$

Relación de Reflujo

$$R = 3.5$$

Flujo molar LD

$$L_D = 490\ \frac{\text{kmol}}{\text{hr}}$$

Flujo molar VD

$$V_D = 630\ \frac{\text{kmol}}{\text{hr}}$$

Balance de materia para la zona de Agotamiento "Rehervidor"

$$S = \frac{V}{B} \qquad L_B := B + V_B \qquad S := \frac{V_B}{B}$$

Relación de Re-ebullición

$$S = 3$$

Flujo molar LB

$$L_B = 840\ \frac{\text{kmol}}{\text{hr}}$$

Flujo molar VB

$$V_B = 630\ \frac{\text{kmol}}{\text{hr}}$$

Point Pinch

$$x_{int} := 1 \qquad x_0 := z \qquad y_0 := x_0 \qquad x_1 := (1 - z) \qquad y_1 := \frac{q}{q-1} \cdot x_1 - \frac{z}{q-1}$$

$$x_{pinch} := \left(\text{solve}\left(\left(y_0 + \frac{y_1 - y_0}{x_1 - x_0} \cdot \left(x_{int} - x_0 \right) \right) - \text{cinterp}\left(X , Y , x_{int} \right) , x_{int} , 0 , 1 \right) \right) = 0.5063$$

$$y_{pinch} := \text{cinterp}\left(X , Y , x_{pinch} \right) = 0.71886642683001$$

$$y_{LR} := 0 \cdot \frac{R}{1+R} + \frac{x_D}{1+R} = 0.2156$$

$$Y_{LA} := 1 \cdot \frac{R \cdot \left(z - x_B \right) + q \cdot \left(x_D - x_B \right)}{q \cdot \left(x_D - x_B \right) + R \cdot \left(z - x_B \right) - x_D + z} + \frac{x_B \cdot \left(z - x_D \right)}{q \cdot \left(x_D - x_B \right) + R \cdot \left(z - x_B \right) - x_D + z} = 1.2557$$

$$I(x) := \text{linterp}\left(\begin{bmatrix} z \\ x_{pinch} \end{bmatrix} , \begin{bmatrix} z \\ y_{pinch} \end{bmatrix} , x \right) \qquad II(x) := \text{linterp}\left(\begin{bmatrix} x_B \\ 1 \end{bmatrix} , \begin{bmatrix} x_B \\ Y_{LA} \end{bmatrix} , x \right)$$

$$x_{LO} := \left(\text{solve}\left(I(x) = II(x) , x , 0 , 1 \right) \right) = 0.457$$

$$y_{LO} := I\left(x_{LO} \right) = 0.57099999832695$$

$$y_{Interpolado} := \text{linterp}\left(X , Y , x_{LO} \right) = 0.6743$$

Funciones

$$LA(x) := \frac{q}{q-1} \cdot x - \frac{z}{q-1}$$

$$LOSE(x) := x \cdot \frac{R}{1+R} + \frac{x_D}{1+R}$$

$$LOSA(x) := x \cdot \frac{R \cdot (z - x_B) + q \cdot (x_D - x_B)}{q \cdot (x_D - x_B) + R \cdot (z - x_B) - x_D + z} + \frac{x_B \cdot (z - x_D)}{q \cdot (x_D - x_B) + R \cdot (z - x_B) - x_D + z}$$

$$LO(x) := \begin{cases} \text{if } x < \dfrac{x_D \cdot (q-1) + z \cdot (R+1)}{q+R} \\ \quad LOSA(x) \\ \text{else} \\ \quad LOSE(x) \end{cases}$$

$$G(x) := \text{cinterp}(X, Y, x)$$

McCabe Codigo

$$McCabe_{ER} := \begin{array}{l} \text{if } y_{LO} \geq y_{Interpolado} \\ \quad \text{"No es posible trazar el gráfico. Cambia q ó diminuye la presión"} \\ \text{else} \\ \quad x_{propuesta} := 0 \\ \quad x_1 := x_D \\ \quad y_1 := x_D \\ \quad x_2 := \text{solve}\left(G\left(x_{propuesta}\right) - y_1, x_{propuesta}, 0, 1\right) \\ \quad y_2 := y_1 \\ \quad i := 3 \\ \quad \text{while } x_{i-2} > x_B \\ \quad\quad x_{i-1} := x_{i-2} \\ \quad\quad y_{i-1} := LO\left(x_{i-1}\right) \\ \quad\quad x_i := \text{solve}\left(G\left(x_{propuesta}\right) - y_{i-1}, x_{propuesta}, 0, 1\right) \\ \quad\quad y_i := y_{i-1} \\ \quad\quad i := i + 2 \\ \quad x_{i-1} := x_{i-2} \\ \quad y_{i-1} := x_{i-2} \\ \quad \text{augment}(x, y) \end{array}$$

$ER =$ "Etapas Requeridas" $\quad ER := McCabe_{ER}$

$xer := \text{col}(ER, 1) \quad yer := \text{col}(ER, 2)$

$$Etapas := \left\lfloor \frac{\text{rows}(xer)}{2} \right\rfloor - 1$$

$Titulo := [\text{"Coordenada X"} \ \text{"Coordenada Y"}]$

$$\text{McCabe}_{\text{mín}} := \left| \begin{array}{l} x_{\text{propuesta}} := 0 \\ x_1 := x_D \\ y_1 := x_D \\ x_2 := \text{solve}\left(G\left(x_{\text{propuesta}}\right) - y_1, x_{\text{propuesta}}, 0, 1\right) \\ y_2 := y_1 \\ i := 3 \\ \text{while } x_{i-2} > x_B \\ \quad \left| \begin{array}{l} x_{i-1} := x_{i-2} \\ y_{i-1} := x_{i-1} \\ x_i := \text{solve}\left(G\left(x_{\text{propuesta}}\right) - y_{i-1}, x_{\text{propuesta}}, 0, 1\right) \\ y_i := y_{i-1} \\ i := i + 2 \end{array} \right. \\ x_{i-1} := x_{i-2} \\ y_{i-1} := x_{i-2} \\ \text{augment}(x, y) \end{array} \right.$$

$$E_{\text{mín}} = \text{"Etapas mínimas"}$$

$$E_{\text{mín}} := \text{McCabe}_{\text{mín}}$$

$$\text{xer}_{\text{mín}} := \text{col}\left(E_{\text{mín}}, 1\right)$$

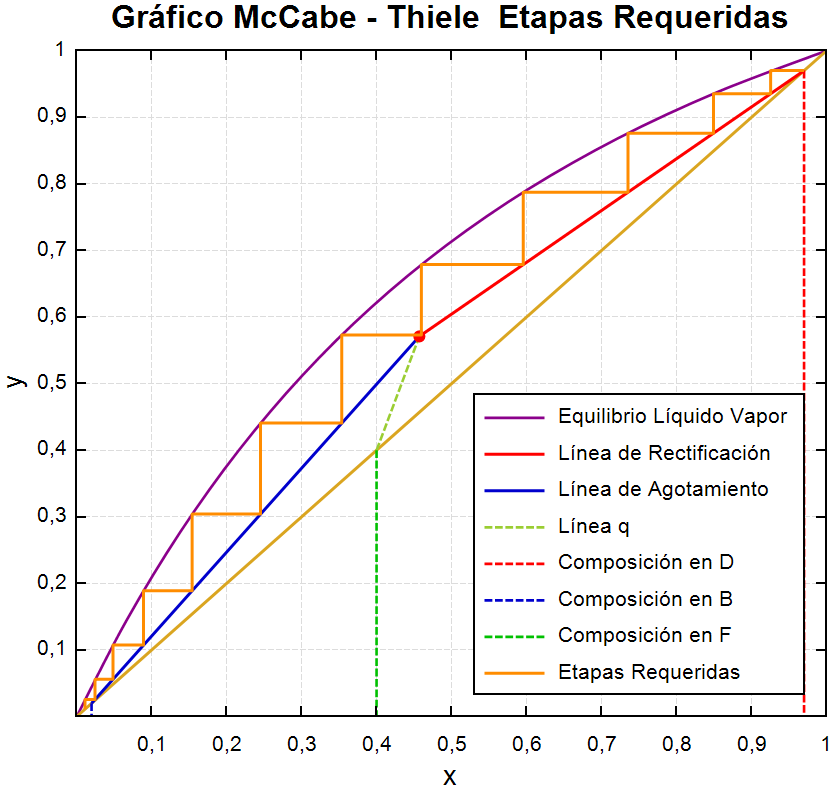
$$\text{yer}_{\text{mín}} := \text{col}\left(E_{\text{mín}}, 2\right)$$

$$E_{\text{mínimas}} := \left| \frac{\text{rows}\left(\text{xer}_{\text{mín}}\right)}{2} \right| - 1$$

Notas:

*Si el diagrama McCabe no se traza o el punto "Rojo" sale o toca la curva del Equilibrio Líquido - Vapor, debes cambiar "q" o disminuir la presión.

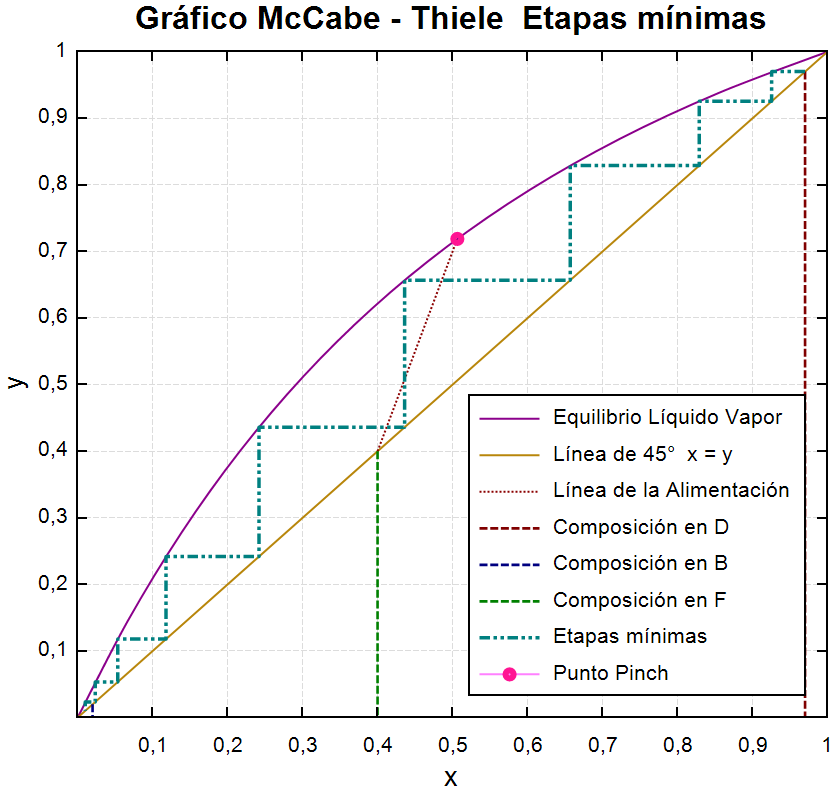
Número de Etapas Requeridas $Etapas = 12$



Número de Etapas mínimas $E_{mínimas} = 9$

$$m := \frac{x_D - y_{pinch}}{x_D - x_{pinch}} \qquad R_{mín} := \frac{m}{1 - m}$$

$R_{mín} = 1.1814$ Relación de Reflujo mínimo



Coordenadas del punto pinch

$$Coordenadas_{Pinch} := \left[x_{pinch} \; y_{pinch} \right]$$

Coordenadas Punto Pinch	
Coordenada X	Coordenada Y
0.506	0.719

Coordenadas del punto de intersección de las líneas de operación

$$Coordenadas_{LO} := \left[x_{LO} \; y_{LO} \right]$$

Intersección en L. de Operación	
Coordenada X	Coordenada Y
0.457	0.571

Coordenadas de los puntos de las etapas requeridas del McCabe-Thiele

Etapas McCabe - Thiele	
Coordenada X	Coordenada Y
0.970	0.970
0.970	0.970
0.925	0.970
0.925	0.935
0.849	0.935
0.849	0.876
0.735	0.876
0.735	0.787
0.596	0.787
0.596	0.679
...	

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