



Solubility of syngas components in water acetic acid and alcohol using new standard fugacity methodology

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Supporting information

In the tables below, from 1 to 15, are listed the number of points involved in the final model parameter estimation and the number of relevant experimental measurement reported in the original papers. Concentration intervals, temperature and pressure ranges are included as well.

Table 1: Literature data for CO₂-H₂O system in different experimental ranges

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
6.30·10 ⁻⁴ -2.26·10 ⁻²	298-448	10.9-175.3	38	1
4.99·10 ⁻⁴ -2.58·10 ⁻²	289-533	6.9-202.7	29(30)	2
5.13·10 ⁻⁴ -7.55·10 ⁻⁴	290-303	atmospheric	14	3
2.53·10 ⁻⁴ -6.83·10 ⁻⁴	303-333	atmospheric	1(7)	4
2.64·10 ⁻⁵ -8.26·10 ⁻⁴	285-350	0.13-0.97	49(54)	5
8.00·10 ⁻³ -2.98·10 ⁻¹	323-623	200-3500	12(104) ^{b,c}	6
4.00·10 ⁻³ -2.50·10 ⁻¹	383-623	100-1500	20(116) ^{b,c}	7
5.00·10 ⁻⁴ -7.60·10 ⁻³	323-473	1.5-53.9	33	8
1.65·10 ⁻² -2.26·10 ⁻²	323	68.2-176.8	8	9
3.90·10 ⁻⁴ -1.03·10 ⁻²	373-473	3.2-81.1	49	10
1.54·10 ⁻² -2.04·10 ⁻²	348-421	101.8-197.2	5(7)	11
4.60·10 ⁻³ -2.15·10 ⁻²	304-313	10.1-60.8	17(20)	12
8.00·10 ⁻³ -2.17·10 ⁻²	323-353	40.5-141.1	29	13
1.82·10 ⁻³ -2.80·10 ⁻²	278-318	4.6-79.6	47	14
3.80·10 ⁻⁴ -3.65·10 ⁻³	288-323	0.92-4.7	47(49)	15
6.40·10 ⁻³ -2.27·10 ⁻²	323-373	20.6-202.0	8	16
2.00·10 ⁻⁴ -3.32·10 ⁻³	298-335	0.60-5.3	17(50)	17
3.75·10 ⁻⁴ -9.12·10 ⁻³	313-333	1.2-25.1	12(17)	18
1.26·10 ⁻³ -2.22·10 ⁻²	298-393	5.4-51.4	30	19
4.00·10 ⁻⁴ -2.30·10 ⁻³	298-323	1.2-4.1	9	20
8.53·10 ⁻³ -2.64·10 ⁻²	273-298	10.1-45.6	6(12)	21
1.56·10 ⁻² -2.10·10 ⁻²	323-348	101.3-152.0	4	22
2.20·10 ⁻³ -1.66·10 ⁻²	353-471	20.4-102.1	30(33)	23
1.40·10 ⁻² -2.70·10 ⁻²	313	40-100	2	24
2.08·10 ⁻² -2.51·10 ⁻²	323	101-310	2(3)	25
1.63·10 ⁻⁴ -5.69·10 ⁻⁴	278-338	0.49-0.84	10	26
1.56·10 ⁻² -2.34·10 ⁻²	278-283	20.0-37.0	5(6)	27
6.60·10 ⁻³ -1.47·10 ⁻²	293	10.1-25.3	4	28
7.64·10 ⁻³ -1.26·10 ⁻²	297-370	15.5-83.4	26	29
4.96·10 ⁻³ -1.80·10 ⁻²	304-313	10.1-45.9	6(8)	30
3.98·10 ⁻⁴ -6.87·10 ⁻⁴	293-313	atmospheric	4	31
1.53·10 ⁻² -3.02·10 ⁻⁴	324-376	106-499	3(7) ^c	32
1.34·10 ⁻² -2.46·10 ⁻²	353-393	100-300	5	33
1.70·10 ⁻³ -4.60·10 ⁻³	298-299	2.6-7.5	6(7)	34
1.10·10 ⁻² -2.19·10 ⁻²	374-375	72.1-272.6	5	35
3.52·10 ⁻³ -1.54·10 ⁻²	323	10.6-58.0	7	36
5.17·10 ⁻³ -2.62·10 ⁻²	293-373	20-167	29(55)	37
4.49·10 ⁻⁴ -6.63·10 ⁻⁴	293-307	atmospheric	8	38
2.77·10 ⁻³ -1.64·10 ⁻²	293-303	4.9-29.4	8(9)	39
4.10·10 ⁻³ -3.02·10 ⁻²	323-373	25-709	20(29) ^c	40
9.32·10 ⁻³ -2.98·10 ⁻²	291-313	25-506	15(22) ^f	41
3.11·10 ⁻⁴ -1.38·10 ⁻³	273-323	atmospheric	18	42
1.52·10 ⁻⁴ -8.43·10 ⁻⁴	286-348	atmospheric	19	43
2.24·10 ⁻³ -2.12·10 ⁻²	450-607	25.2-198.7	10(15) ^b	44
1.97·10 ⁻³ -1.70·10 ⁻²	303-353	9.3-39.3	13	45
4.54·10 ⁻⁴ -1.32·10 ⁻³	274-308	atmospheric	8	46
3.00·10 ⁻⁵ -2.48·10 ⁻²	313-393	0.95-92.6	18(39)	47
5.38·10 ⁻⁴ -1.64·10 ⁻²	283-303	1.0-20.3	15	48
1.07·10 ⁻² -5.42·10 ⁻²	298-423	100-800	6(17) ^c	49
3.80·10 ⁻³ -3.00·10 ⁻²	374-393	23-703	15(26) ^c	50
4.30·10 ⁻³ -3.20·10 ⁻²	285-373	25-709	43(72) ^c	51
5.90·10 ⁻⁴ -1.08·10 ⁻³	298	0.99-1.80	10	52
6.06·10 ⁻⁴ -1.08·10 ⁻³	298	1.01-1.80	12	53
2.09·10 ⁻⁴ -6.09·10 ⁻⁴	298	0.35-1.02	8(10)	54
2.18·10 ⁻⁴ -7.90·10 ⁻⁴	298	0.36-1.32	15(18)	55
7.13·10 ⁻⁴ -1.44·10 ⁻³	273-293	atmospheric	21	56 ^d
7.64·10 ⁻⁴ -3.63·10 ⁻³	288	0.93-4.1	1(10)	56 ^e
2.28·10 ⁻⁴ -1.37·10 ⁻³	273-335	atmospheric	15	56 ^f
5.69·10 ⁻⁴ -7.44·10 ⁻⁴	293-294	atmospheric	13(14)	56 ^g
3.46·10 ⁻³ -2.64·10 ⁻²	273-373	10.8-94.5	57(60)	56 ^h
9.93·10 ⁻⁵ -1.26·10 ⁻⁴	291-295	0.15-0.20	1(6)	56 ⁱ
1.07·10 ⁻² -1.28·10 ⁻¹	473-603	98-490	31(79) ^{b,c}	56 ^j
8.10·10 ⁻³ -2.14·10 ⁻²	293-308	25.3-76.0	3(20)	56 ^k
1.16·10 ⁻² -5.82·10 ⁻²	323-423	100-800	6(14) ^c	56 ^l
2.72·10 ⁻³ -7.17·10 ⁻³	306-486	8.0-58.0	7	56 ^m

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above the maximum temperature considered of 90% of the solvent critical temperature

^cPoints discarded when above the maximum pressure considered of 400 bar

^dVerdet (1855), ^ede Khanikof & Louguinine (1867), ^fBohr (1899), ^gBuch (1926), ^hZel'venskii (1937), ⁱKoch et al. (1949), ^jMalinin (1959), ^kVilcu and Gainar (1967), ^lShagiakhmetov & Tarzimanov (1982), ^mCramer(1982)

Table 2: Literature data for CO₂-C₂H₅OH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
3.28·10 ⁻³ -3.43·10 ⁻²	288-323	0.86-5.38	20(23)	15
1.09·10 ⁻¹ -3.58·10 ⁻¹	293-373	29.4-127.5	7(24)	37
5.40·10 ⁻³ -7.13·10 ⁻³	291-307	atmospheric	9	38
2.66·10 ⁻¹ -9.50·10 ⁻¹	313-343	50.3-118.0	10(29)	57
1.90·10 ⁻¹ -9.97·10 ⁻¹	304-323	33.1-79.6	23(30)	58
1.87·10 ⁻² -9.29·10 ⁻¹	313-333	5.3-106.3	16(24)	59
2.00·10 ⁻² -8.73·10 ⁻¹	313-333	5.1-106.5	12(23)	60
2.73·10 ⁻¹ -9.96·10 ⁻¹	304-308	37.5-76.7	6(19)	61
1.83·10 ⁻¹ -8.86·10 ⁻¹	305-323	22.2-91.7	27(33)	62
1.14·10 ⁻¹ -8.76·10 ⁻¹	298	15.5-59.0	18	63
5.29·10 ⁻² -8.30·10 ⁻¹	291-313	8.6-79.2	45(68)	64
1.10·10 ⁻¹ -9.95·10 ⁻¹	308	15.5-77.9	10(20)	65
3.30·10 ⁻² -9.70·10 ⁻¹	312	6-81.5	5(11)	66
2.72·10 ⁻¹ -8.45·10 ⁻¹	315-337	55.5-108.4	16(23)	67
5.29·10 ⁻² -8.49·10 ⁻¹	291-313	9.1-79.2	37(60)	68
1.21·10 ⁻¹ -9.08·10 ⁻¹	303-329	17.8-91.0	39(52)	69
2.90·10 ⁻² -8.50·10 ⁻¹	323-329	13.2-146.2	11(22)	70
2.48·10 ⁻¹ -5.09·10 ⁻¹	323	50.3-82.0	12	71
2.85·10 ⁻² -6.43·10 ⁻¹	323-333	7.3-94.6	13(22)	72
2.37·10 ⁻² -9.46·10 ⁻¹	313-373	4.8-141.1	23(43)	73
2.69·10 ⁻² -9.67·10 ⁻¹	313-345	5.7-119.3	20(55)	74
7.26·10 ⁻² -8.13·10 ⁻¹	333-453	40.0-145.0	10(21)	75
5.40·10 ⁻² -6.10·10 ⁻¹	348-368	20.0-140.0	1(7)	76
7.78·10 ⁻² -8.44·10 ⁻¹	313-328	16.0-94.2	12(22)	77
1.34·10 ⁻¹ -7.81·10 ⁻¹	333	30.5-104.1	4(7)	78
1.84·10 ⁻¹ -9.96·10 ⁻¹	291	20.9-54.0	9	79
5.50·10 ⁻³ -3.28·10 ⁻¹	288-318	0.6-57.3	62(70)	80
2.00·10 ⁻¹ -8.00·10 ⁻¹	333-483	70.0-142.4	26(59) ^b	81
1.92·10 ⁻¹ -9.85·10 ⁻¹	291-313	24.5-81.8	45(64)	82
5.78·10 ⁻² -7.55·10 ⁻¹	313-353	13.1-139.0	11(31)	83
1.87·10 ⁻² -9.13·10 ⁻¹	293-353	5.2-110.8	36(46)	84
4.80·10 ⁻² -7.26·10 ⁻¹	313	6.1-77.2	15(16)	85
1.00·10 ⁻¹ -9.50·10 ⁻¹	313	19.7-81.8	6(10)	86
2.70·10 ⁻² -2.12·10 ⁻¹	313	5.1-38.1	8	87
5.98·10 ⁻² -7.70·10 ⁻¹	333-373	11.2-141.5	31(36)	88
4.90·10 ⁻² -5.89·10 ⁻¹	303-323	10.2-60.8	11(12)	89
5.55·10 ⁻² -2.19·10 ⁻¹	293-303	7.5-30.5	6	90
5.30·10 ⁻² -2.06·10 ⁻¹	293-303	7.2-29.0	6	91
5.86·10 ⁻³ -7.45·10 ⁻³	288-298	atmospheric	3	92
5.97·10 ⁻¹ -9.56·10 ⁻¹	298-409	61.8-151.7	1(15)	93
2.41·10 ⁻¹ -4.86·10 ⁻¹	291-323	33.0-81.1	11(12)	94
5.50·10 ⁻¹ -9.50·10 ⁻¹	314-324	70.7-83.0	3(7)	95
6.60·10 ⁻¹ -8.20·10 ⁻¹	238-308	8.6-71.4	15(17)	96
3.37·10 ⁻¹ -8.75·10 ⁻¹	314	55.4-79.2	5(8)	97
2.20·10 ⁻¹ -5.36·10 ⁻¹	373	70.0-133.0	1(3)	98
2.07·10 ⁻¹ -8.07·10 ⁻¹	298-323	27.9-88.9	21(28)	99
6.80·10 ⁻³ -7.57·10 ⁻³	290-296	atmospheric	6	100 ^c
4.35·10 ⁻³ -1.05·10 ⁻²	278-333	1.04-1.49	3(7)	100 ^d

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above the maximum temperature considered of 90% of the solvent critical temperature

^cKosakewitsch (1929), ^dCargill and MacPhee (1981)

Table 3: Literature data for CO₂-CH₃COOH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points	Reference
4.85·10 ⁻¹ -7.98·10 ⁻¹	323	56.2-83.7	5	9
9.64·10 ⁻² -7.10·10 ⁻¹	313-353	11.0-111.0	20	13
9.16·10 ⁻³ -1.28·10 ⁻²	291-309	atmospheric	10	38
1.07·10 ⁻² -1.32·10 ⁻²	288-298	atmospheric	3	92
1.20·10 ⁻² -7.54·10 ⁻¹	298-348	2.7-74.1	50	101
7.93·10 ⁻² -8.18·10 ⁻¹	293-333	6.4-74.3	19	102
5.04·10 ⁻¹	283-364	29.0-103.3	9	103

Table 4: Literature data for CO-H₂O system

Gas solubility mol frac	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
1.84·10 ⁻⁵ -2.03·10 ⁻⁵	293-298	atmospheric	2	92
1.63·10 ⁻⁵ -2.85·10 ⁻⁵	273-303	atmospheric	19	104
1.02·10 ⁻⁵ -2.72·10 ⁻⁵	273-353	0.63-1.61	47	105
3.43·10 ⁻⁴ -4.15·10 ⁻⁴	343-403	32	7	106
1.21·10 ⁻⁴ -1.27·10 ⁻³	298-573	11.3-94.29	84 (118) ^b	107
2.97·10 ⁻⁵ -3.34·10 ⁻³	311-589	3.4-137.9	17(18) ^b	108
2.91·10 ⁻⁴ -1.17·10 ⁻³	298-448	20.3-72.2	4(12)	109
8.92·10 ⁻⁶ -2.08·10 ⁻⁵	278-323	0.59-1.09	14	110
7.49·10 ⁻⁶ -2.83·10 ⁻⁵	273-353	atmospheric	8	111
6.22·10 ⁻⁶ -1.45·10 ⁻⁵	310	0.48-1.01	15	112
1.43·10 ⁻⁵ -2.18·10 ⁻⁵	285-310	atmospheric	3	112
1.80·10 ⁻⁵ -2.28·10 ⁻⁵	279-295	atmospheric	6	113c

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above 250 °C. According to Jung and Knacke¹⁰⁷, above this temperature the water gas shift reaction (WGS) becomes kinetically active altering the system composition

^cBunsen (1855)

Table 5: Literature data for CO-C₂H₅OH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
4.61·10 ⁻⁴	293-298	atmospheric	2	92
9.72·10 ⁻³ -4.59·10 ⁻²	298-448	20.3-83.17	12	109
5.00·10 ⁻³ -2.21·10 ⁻²	298-323	10.1-40.3	8	114
4.85·10 ⁻⁴ -4.94·10 ⁻⁴	293-323	atmospheric	10	115
5.88·10 ⁻³ -1.72·10 ⁻²	373-413	11.0-24.4	2(6)	116
4.61·10 ⁻⁴	298	atmospheric	1	117

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

Table 6: Literature data for CO-CH₃COOH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points	Reference
3.95·10 ⁻⁴ -3.96·10 ⁻⁴	293-298	atmospheric	2	92
9.00·10 ⁻⁴ -2.07·10 ⁻²	298-348	2.2-55.6	42	101
6.79·10 ⁻³ -3.10·10 ⁻²	298-448	20.3-70.3	12	109
3.97·10 ⁻⁴ -4.00·10 ⁻⁴	298	atmospheric	2	117

Table 7: Literature data for CH₄-H₂O system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
1.73·10 ⁻⁴ -6.76·10 ⁻³	323-589	1308-168.9	12(16)	2
1.48·10 ⁻³ -2.74·10 ⁻³	298	73.6-178.2	4	28
8.65·10 ⁻⁶ -5.26·10 ⁻⁵	285-348	atmospheric	7(11)	43
1.34·10 ⁻⁵ -2.59·10 ⁻⁵	273-353	0.58-1.44	38	105
5.10·10 ⁻⁴ -1.62·10 ⁻³	298-323	30-80	6	118
2.54·10 ⁻⁵ -4.03·10 ⁻⁵	278-298	atmospheric	5	119
6.04·10 ⁻⁴ -2.61·10 ⁻³	284-324	47.8-194.9	17(22)	120
9.10·10 ⁻⁶ -2.60·10 ⁻⁴	303-323	1.12-6.38	1(18)	121
5.63·10 ⁻⁴ -4.05·10 ⁻³	283-303	20-400	16(17)	122
2.04·10 ⁻⁴ -2.46·10 ⁻³	275-313	9.7-180.0	16	123
2.10·10 ⁻⁴ -1.60·10 ⁻³	299-314	9.9-99.8	8	124
1.49·10 ⁻⁵ -4.32·10 ⁻⁵	275-328	0.82-1.18	16	125
1.79·10 ⁻⁵ -2.76·10 ⁻⁵	293-323	1.04-1.14	13	126
7.41·10 ⁻⁴ -1.09·10 ⁻¹	427-627	35-1972	10(71) ^{b,c}	127
8.87·10 ⁻⁴ -4.11·10 ⁻³	324-375	56-580	7(14) ^c	128
6.00·10 ⁻⁵ -1.13·10 ⁻³	298-303	3.2-51.7	14(17)	129
1.40·10 ⁻³ -4.10·10 ⁻³	324-376	109-499	4(7) ^c	130
3.23·10 ⁻⁴ -7.75·10 ⁻³	298-444	22-689	55(71) ^c	131
1.36·10 ⁻³ -4.30·10 ⁻³	325-398	101-616	18(28) ^c	132
2.76·10 ⁻⁴ -1.53·10 ⁻³	283-298	11.3-51.8	21	133
2.58·10 ⁻⁴ -2.00·10 ⁻³	274-286	5.7-90.8	16(18)	134
4.05·10 ⁻⁴ -2.21·10 ⁻³	298-338	25.0-125.0	15	135
1.47·10 ⁻⁵ -4.61·10 ⁻⁵	273-358	1.02-1.59	18	136
1.44·10 ⁻³ -3.41·10 ⁻³	324	100-400	3(4)	137
1.90·10 ⁻⁵ -3.98·10 ⁻⁵	278-318	atmospheric	9	138
6.40·10 ⁻⁵ -6.35·10 ⁻⁴	311-394	3.5-38.4	45(46)	139
2.13·10 ⁻⁵ -3.98·10 ⁻⁵	278-308	atmospheric	4	140
1.08·10 ⁻³ -2.11·10 ⁻³	273-285	26.5-91.0	13	141
2.12·10 ⁻⁴ -1.03·10 ⁻³	298-518	13.3-64.5	7	142
9.00·10 ⁻⁵ -4.26·10 ⁻³	298	4-468	22(34) ^c	143
5.00·10 ⁻⁵ -1.54·10 ⁻³	313-373	3.4-92.6	26	144
9.58·10 ⁻⁴ -2.44·10 ⁻³	298	37.7-115.1	2(4)	145
6.10·10 ⁻⁴ -2.97·10 ⁻³	298-423	41-469	13(39) ^c	146
2.25·10 ⁻⁵ -4.47·10 ⁻⁵	274-303	atmospheric	35	147
2.22·10 ⁻⁴ -1.24·10 ⁻³	303-373	9.7-71.3	91(167)	148
1.75·10 ⁻⁵ -3.93·10 ⁻⁵	278-318	atmospheric	3	149
1.78·10 ⁻⁵ -4.35·10 ⁻⁵	275-313	atmospheric	6	150
2.33·10 ⁻⁵ -3.47·10 ⁻⁵	283-303	atmospheric	5	151
1.97·10 ⁻⁵ -2.80·10 ⁻⁵	291-310	atmospheric	6	152 ^d
1.00·10 ⁻³ -1.43·10 ⁻¹	423-633	98-1132	5 (56) ^{b,c}	152 ^e

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above the maximum temperature considered of 90% of the solvent critical temperature

^cPoints discarded when above the maximum pressure considered of 400 bar

^dLannung and Gjaldbaek (1960), ^eSultanov et al. (1972)

Table 8: Literature data for CH₄-C₂H₅OH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
2.10·10 ⁻² -1.07·10 ⁻¹	313-333	18.1-104.6	10	60
9.50·10 ⁻³ -1.05·10 ⁻¹	298	10.0-120.0	5	145
1.20·10 ⁻³ -1.33·10 ⁻³	291-310	atmospheric	6	152 ^b
1.00·10 ⁻³ -1.11·10 ⁻³	293-313	atmospheric	3	153
1.23·10 ⁻³ -1.38·10 ⁻³	283-303	atmospheric	5	154
2.30·10 ⁻² -1.24·10 ⁻¹	280-333	21.0-121.0	19	155
1.80·10 ⁻² -1.26·10 ⁻¹	280	15.7-113.7	10	156
1.30·10 ⁻² -9.90·10 ⁻²	295	10.2-79.9	7(8)	157
2.36·10 ⁻² -2.70·10 ⁻²	323-373	21.2-26.6	3(4)	158
2.44·10 ⁻² -4.35·10 ⁻¹	298-498	33.2-315.3	14(27)	159
1.22·10 ⁻³	298	atmospheric	1	160
1.28·10 ⁻³	298	atmospheric	1	161

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bLannung and Gjaldbaek (1960)

Table 9: Literature data for CH₄-CH₃COOH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points	Reference
1.20·10 ⁻³ -3.82·10 ⁻²	298-348	2.6-70.2	43	101

Table 10: Literature data for N₂-H₂O system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
5.38·10 ⁻⁶ -1.36·10 ⁻⁵	286-346	atmospheric	12	43
1.15·10 ⁻⁵ -1.83·10 ⁻⁵	274-304	atmospheric	10	46
2.30·10 ⁻⁵ -2.94·10 ⁻³	311-589	3.4-137.9	12(16)	108
9.26·10 ⁻⁶ -1.68·10 ⁻⁵	278-313	atmospheric	8	138
2.06·10 ⁻⁴ -4.05·10 ⁻⁴	298	20.3-40.6	2	145
1.30·10 ⁻⁴ -5.86·10 ⁻⁴	313-363	9.0-60.8	54(94)	148
1.07·10 ⁻⁵ -1.55·10 ⁻⁵	283-298	0.84	3(4)	162
7.40·10 ⁻⁵ -1.07·10 ⁻³	274-363	9.1-71.6	52	163
3.22·10 ⁻⁶ -1.70·10 ⁻³	273-433	1.0-200.0	48(85)	164
9.64·10 ⁻⁶ -1.77·10 ⁻⁵	276-310	atmospheric	6	165
7.84·10 ⁻⁶ -1.86·10 ⁻⁵	274-325	atmospheric	25	166
1.15·10 ⁻⁵	298	atmospheric	1	167
1.11·10 ⁻⁵ -1.83·10 ⁻⁵	275-300	atmospheric	33	168
1.23·10 ⁻⁵	294	atmospheric	1	169
2.10·10 ⁻⁴ -5.71·10 ⁻³	298-373	25-1013	20(24) ^b	170

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above the maximum pressure considered of 400 bar

Table B 11: Literature data for N₂-C₂H₅OH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
3.17·10 ⁻⁴ -3.20·10 ⁻⁴	293-298	atmospheric	2	92
3.62·10 ⁻⁴	298	atmospheric	1	116
1.25·10 ⁻² -2.74·10 ⁻²	323-373	35.0-70.0	6	158
3.51·10 ⁻⁴	298	atmospheric	1	160
3.48·10 ⁻⁴	298	atmospheric	1	161
2.60·10 ⁻⁴ -4.36·10 ⁻²	298-398	0.8-98.7	36	171
2.98·10 ⁻⁴ -3.45·10 ⁻⁴	293-313	atmospheric	2	172
2.97·10 ⁻⁴ -3.46·10 ⁻⁴	273-313	atmospheric	3	173
2.59·10 ⁻⁴ -3.49·10 ⁻⁴	248-323	atmospheric	4	174
3.29·10 ⁻⁴ -3.70·10 ⁻⁴	213-298	atmospheric	4(5)	175

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

Table 12: Literature data for N₂-CH₃COOH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points	Reference
2.75·10 ⁻⁴ -2.74·10 ⁻⁴	293-298	atmospheric	2	92
1.00·10 ⁻³ -2.67·10 ⁻²	323-473	10.1-60.8	25	176

Table 13: Literature data for H₂-H₂O system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
1.29·10 ⁻⁵ -1.55·10 ⁻⁵	285-345	atmospheric	10(12)	43
3.74·10 ⁻⁵ -2.98·10 ⁻³	311-589	3.4-137.9	17(18) ^b	108
6.56·10 ⁻⁴ -2.05·10 ⁻³	298	50.3-152.3	5	145
1.98·10 ⁻⁴ -1.72·10 ⁻³	293-408	10-3-99.8	75(114)	148
2.00·10 ⁻⁴ -2.71·10 ⁻³	366-589	13.8-110.3	8(9) ^b	177
1.31·10 ⁻⁵ -1.38·10 ⁻⁵	298-353	atmospheric	3(4)	178
1.36·10 ⁻⁵	298	atmospheric	1	179
4.02·10 ⁻⁴ -2.23·10 ⁻³	323-423	31.8-153.7	10	180
1.39·10 ⁻⁵ -1.70·10 ⁻⁵	275-299	atmospheric	5	181
1.15·10 ⁻⁵ -1.70·10 ⁻⁵	274-323	atmospheric	6	182
1.38·10 ⁻⁵ -1.49·10 ⁻⁵	288-298	atmospheric	2	183
1.30·10 ⁻⁵ -1.47·10 ⁻⁵	292-305	atmospheric	3	184
1.31·10 ⁻⁵ -1.32·10 ⁻⁵	303	atmospheric	4	185
1.05·10 ⁻⁵ -1.39·10 ⁻⁵	298-333	atmospheric	3	186
1.32·10 ⁻⁵ -1.72·10 ⁻⁵	275-302	atmospheric	42 ^b	187
1.33·10 ⁻⁵ -1.77·10 ⁻⁵	373-302	atmospheric	6	188
3.50·10 ⁻⁴ -1.21·10 ⁻²	298	25-1013	5(8) ^c	189
3.27·10 ⁻⁴ -1.43·10 ⁻²	273-373	25-1013	21(48) ^c	190
2.65·10 ⁻⁴ -1.61·10 ⁻³	325-616	13.9-161.0	4(13) ^b	191
4.28·10 ⁻⁵ -1.64·10 ⁻²	319-636	4.4-284.5	20(26) ^b	192
2.46·10 ⁻⁴ -2.02·10 ⁻³	373-436	16.5-101.3	47(48)	193
1.42·10 ⁻⁵	293	atmospheric	1	194 ^d

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above the maximum temperature considered of 90% of the solvent critical temperature

^cPoints discarded when above the maximum pressure considered of 400 bar

^dHufner

Table 14: Literature data for H₂-C₂H₅OH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
1.05·10 ⁻² -4.11·10 ⁻¹	298-508	41.0-333.0	19(35) ^b	159
1.16·10 ⁻⁴ -1.95·10 ⁻⁴	213-293	atmospheric	2(5)	175
1.63·10 ⁻⁴ -1.82·10 ⁻⁴	298-323	atmospheric	2	179
3.10·10 ⁻³ -6.70·10 ⁻³	291	13.9-31.2	4	195
1.28·10 ⁻⁴ -1.91·10 ⁻⁴	279-333	atmospheric	6	196
1.67·10 ⁻⁴ -1.92·10 ⁻⁴	274-323	atmospheric	8	197

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

^bPoints discarded when above the maximum temperature considered of 90% of the solvent critical temperature

Table 15: Literature data for H₂-CH₃COOH system

Gas solubility [mol/mol total]	Temperature T[K]	Pressure P[bar]	Data points ^a	Reference
1.20·10 ⁻³ -2.15·10 ⁻²	298-348	2.7-74.5	45(0)	101
1.38·10 ⁻⁴ -1.63·10 ⁻⁴	292-348	atmospheric	11(0)	197
1.45·10 ⁻⁴ -1.46·10 ⁻⁴	293-298	atmospheric	2(0)	92

^aNumbers in parenthesis indicate the total number of relevant experimental data in the paper, in case different from the number of point included in the parameter estimation

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