

Published Modified UNIFAC Interaction Parameters

Literature:

- 1: Weidlich, Gmehling, Ind.Eng.Chem.Res., 26,1372(1987)
- 2: Gmehling, Li, Schiller, Ind.Eng.Chem.Res., 32,178(1993)
- 3: Gmehling, Lohmann, Jakob, Li, Joh, Ind.Eng.Chem.Res., 37,4876-4882(1998)
- 4: Gmehling, Wittig, Lohmann, Joh, Ind.Eng.Chem.Res., 41,1678-1688(2002)
- 5: Wittig, Lohmann, Joh, Horstmann, Gmehling, Ind.Eng.Chem.Res., 40,5831-5838(2001)
- 6: Lohmann, Joh, Gmehling, Ind.Eng.Chem.Res., 40,957-964(2001)
- 7: Lohmann, Gmehling, J.Chem.Eng.Jpn., 34,43-54(2001)
- 8: Wittig, Lohmann, Gmehling, AIChE Journal 49, 2 530-537 (2003)
- 9: Jakob, Grensemann, Lohmann, Gmehling, Ind.Eng.Chem.Res. 45, 7924-7933 (2006)
- 10: Hector, Gmehling, Fluid Phase Equilib. 371, 82-92 (2014)
- 11: Constantinescu, Gmehling, J. Chem. Eng. Data, 61(8), 2738-2748 (2016)

Revised* within the scope of the consortium (available only for members)

Consortium-Parameter (only for members) (Sept. 2017)

*please note that the values displayed in this table are not the consortium parameters



i	j	IP ij	IP ij	IP ij	IP ji	IP ji	IP ji	
1	2	189.66	-0.2723	0.000E+00	-95.418	0.0617	0.000E+00	2
1	3	114.2	0.0933	0.000E+00	16.07	-0.2998	0.000E+00	2
1	4	7.339	-0.4538	0.000E+00	47.2	0.3575	0.000E+00	2
1	5	2777	-4.674	1.551E-03	1606	-4.746	9.181E-04	2
1	6	2409.4	-3.0099	0.000E+00	82.593	-0.4857	0.000E+00	2
1	7	1391.3	-3.6156	1.144E-03	-17.253	0.8389	9.021E-04	2
1	8	1381	-0.9977	0.000E+00	1987	-4.615	0.000E+00	2
1	9	433.6	0.1473	0.000E+00	199	-0.8709	0.000E+00	2
1	10	875.85	0	0.000E+00	256.21	0	0.000E+00	2
1	11	98.656	1.9294	-3.133E-03	632.22	-3.3912	3.928E-03	2
1	12	508.4	-0.6215	0.000E+00	238.5	-0.5358	0.000E+00	2
1	13	233.1	-0.3155	0.000E+00	-9.654	-0.0324	0.000E+00	2
1	14	-164.04	4.9683	-1.025E-02	326.04	-2.6348	3.358E-03	2
1	15	350.58	0.0667	0.000E+00	207.26	-1.0916	0.000E+00	2
1	16	-175.7	1.857	0.000E+00	205.65	-1.4436	0.000E+00	2
1	17	958.74	-0.1484	0.000E+00	2257.3	-5.6676	0.000E+00	2
1	18	1802.3	-17.171	3.600E-02	-436.15	3.4225	-8.700E-03	3
1	19	593.07	0.7335	0.000E+00	293.81	-1.3979	0.000E+00	2
1	20	1182.2	-3.2647	9.198E-03	2017.7	-9.0933	1.024E-02	2
1	21	401	-0.7277	0.000E+00	-65.685	0.0741	0.000E+00	2
1	22	-233.66	1.2561	0.000E+00	311.55	-1.1856	0.000E+00	2
1	23	-653.74	4.5311	-8.735E-03	1302.6	-8.427	1.442E-02	2
1	24	267.51	-1.7109	3.388E-03	-148.07	1.0927	-2.416E-03	2
1	25	-1385	15.89	-4.831E-02	3264	-20.84	3.317E-02	2
1	26	2345	-13.2	2.156E-02	-396.5	3.092	-6.266E-03	2
1	27	2383	-2.693	0.000E+00	1744	-4.082	0.000E+00	2
1	28	24.33	1.521	0.000E+00	72.12	-1.126	0.000E+00	2
1	29	465.9	-0.8557	0.000E+00	-59.9	-0.0083	0.000E+00	2
1	30	577.7	0.9384	0.000E+00	210.5	-1.081	0.000E+00	2
1	31	897.7	0	0.000E+00	28.17	0	0.000E+00	2
1	32	559.9	-0.3564	0.000E+00	166	-0.7116	0.000E+00	2
1	33	527.7	-0.499	0.000E+00	-62.08	-0.3658	0.000E+00	2
1	34	477.5	-0.6581	0.000E+00	-22.04	-0.1018	0.000E+00	2
1	35	-547.5	3.457	0.000E+00	477.1	-2.175	0.000E+00	2
1	36	1662	0	0.000E+00	-291.9	0	0.000E+00	2
1	37	334.5	0.0091	0.000E+00	3.202	-0.6894	0.000E+00	2
1	38	468.5	-1.042	0.000E+00	-160.3	-0.0108	0.000E+00	2
1	39	406.2	0.6525	0.000E+00	151	-0.9023	0.000E+00	2
1	40	342	-1.679	0.000E+00	-484.3	2.467	0.000E+00	2
1	41	1312	-3.643	0.000E+00	-314.6	1.287	0.000E+00	2
1	42	-117.1	0.5481	-9.800E-04	170.9	-0.8062	1.291E-03	3
1	43	79.507	0.7089	-2.098E-03	186.71	-1.3546	2.402E-03	2
1	44	1935.7	0	0.000E+00	-21.23	0	0.000E+00	2
1	45	164.25	-0.2683	0.000E+00	-44.069	0.0278	0.000E+00	2
1	46	677.32	-2.0066	0.000E+00	-249.85	1.7054	0.000E+00	3
1	47	3150.8604	-3.1003	0.000E+00	189.9108	-0.9413	0.000E+00	4
1	48	1529.5217	-6.2025	9.754E-03	82.5982	-0.615	-6.230E-04	5
1	49	-923.28	7.8096	-8.81E-03	183.02	-1.2259	5.83E-04	9
1	50							*
1	51							*
1	52	24.4317	0.2915	0.000E+00	-16.034	-0.5337	0.000E+00	3
1	53	269.6733	0	0.000E+00	-41.0041	0	0.000E+00	6
1	54							*
1	55	407.4698	-0.2037	-1.590E-04	-0.0668	-0.3935	4.100E-05	7
1	56	1058.31	-1.1856	0.000E+00	438.76	-1.2256	0.000E+00	8
1	57							*
1	59							*
1	60							*
1	61	860.51	-1.96	0.000E+00	-309.94	0.6486	0.000E+00	11
1	62							*

2	41	-339.8	1.297	0.000E+00	698.5	-2.159	0.000E+00	2	
2	42	2.406	-0.1882	0.000E+00	60.2	0.1565	0.000E+00	3	
2	43	-322.1	-0.2037	4.517E-03	1182.6	-5	3.745E-03	2	
2	44								*
2	45	389.28	0	0.000E+00	-174.41	0	0.000E+00	2	
2	46	491.23	-1.8285	0.000E+00	-734.87	3.3463	0.000E+00	3	
2	47	673.2267	1.9523	0.000E+00	92.6993	-0.8135	0.000E+00	4	
2	48	249.18	0	0.000E+00	-81.79	0	0.000E+00	4	
2	49	1171.3	3.9213	0.00E+00	90.013	-0.92002	0.00E+00	9	
2	50								*
2	52	-86.2315	0	0.000E+00	-39.3735	0	0.000E+00	3	x
2	53	9.3895	0	0.000E+00	57.8594	0	0.000E+00	6	
2	54								*
2	55	-456.082	2.4334	0.000E+00	298.5526	-1.4153	0.000E+00	7	
2	56	775.56	0	0.000E+00		0	0.000E+00	8	
2	57								*
2	59								*
2	60								*
2	61	324.32	0	0.000E+00	-156.46	0	0.000E+00	11	
2	62								*
2	63								*
2	64								*
2	65								*
2	67								*
2	68								*
2	69								*
2	70								*
2	71								*
2	72								*
2	73								*
2	74								*
2	75								*
2	76								*
2	78								*
2	80								*
2	81								*
2	82								*
2	83								*
2	84	-44.3408	-0.65212	0.000E+00	1753.1349	-3.11209	0.000E+00	2	
2	85	566.2915	-0.14057	0.000E+00	-1213.9299	5.14012	0.000E+00	2	
2	86								*
2	87	-92.7302	-0.25088	0.0000000	-1151.2961	4.7125	0.000E+00	2	
2	88								*
2	89	1230.7809	0.17033	0.0141503	4896.2194	-1.86077	-0.0254894	3	
2	93	-740.24	0	0.000E+00	232.90	0	0.000E+00	11	
2	94								*
2	90	1625.9094	-2.40107	0.000E+00	159.8103	1.85317	0.000E+00	2	*
2	91	2979.9734	4.82369	-0.0272505	724.9113	-4.79411	0.0056279	3	
2	92								*
2	93								*
2	95								*
2	96								*
2	97								*
2	98	2487.6321	-3.28182	0.000E+00	1804.0253	-5.18107	0.000E+00	2	
2	99	-2399.7383	-0.27451	0.0329518	658.1962	0.57714	-0.0078001	3	
2	101								*
2	103								*
2	105								*
2	106								*
3	4	139.2	-0.65	0.000E+00	-45.33	0.4223	0.000E+00	2	
3	5	3972	-13.16	1.208E-02	3049	-12.77	1.435E-02	2	x
3	6	1604.3	-2.0299	0.000E+00	13.733	-0.1177	0.000E+00	2	
3	7	792	-1.726	0.000E+00	332.3	1.158	0.000E+00	2	
3	8	1356	-2.118	0.000E+00	2340	-5.043	0.000E+00	2	x
3	9	146.2	-1.237	4.237E-03	-57.53	1.212	-3.715E-03	2	x
3	10	-365.5	1.874	0.000E+00	1011	-2.167	0.000E+00	2	
3	11	-274.54	0.9149	0.000E+00	622.73	-1.7605	0.000E+00	2	
3	12	170.5	-0.0239	0.000E+00	108.3	-0.262	0.000E+00	2	
3	13	-87.08	-0.1859	0.000E+00	179	0.0562	0.000E+00	2	
3	14	2036	-8.729	8.138E-03	-121	-1.901	6.999E-03	2	
3	15	139.67	0.0377	0.000E+00	105.63	-0.6067	0.000E+00	2	
3	16	-71.4	0.7078	0.000E+00	16.29	-0.6022	0.000E+00	2	
3	17	1044.7	-1.7112	0.000E+00	154.39	1.2458	0.000E+00	2	x
3	18	-1553.9216	0.1615	8.151E-03	1810.7758	-5.7594	2.301E-03	3	x
3	19	-17.44	0.9437	0.000E+00	111.8	-0.5959	0.000E+00	2	
3	20	69.561	1.8881	0.000E+00	613.32	-1.595	0.000E+00	2	
3	21	73.046	-0.2132	0.000E+00	-58.972	0.1046	0.000E+00	2	
3	22	133.66	-0.4614	0.000E+00	-142.2	0.3966	0.000E+00	2	
3	23	66.214	-0.6363	0.000E+00	-78.116	0.6998	0.000E+00	2	
3	24	269	-1.776	2.645E-03	-305.5	2.12	-3.239E-03	2	

7	61	1038.3	0	0.000E+00	-270.53	0	0.000E+00	11		*
7	60									*
7	62									*
7	63									*
7	61	1038.3	0	0.000E+00	-270.53	0	0.000E+00	11		*
7	67									*
7	69									*
7	70									*
7	72									*
7	74									*
7	75									*
7	76									*
7	77									*
7	78									*
7	79									*
7	82									*
7	83									*
7	84	659.2109	-0.59252	0.0451602	151.31	-3.00895	0.0019814	3		
7	85	2770.8505	-2.00944	0.000E+00	1996.7238	-5.47448	0.000E+00	2		
7	88									*
7	89	2707.1611	-2.51124	-0.0022558	-399.1902	0.16195	-0.0067585	3		
7	90	-1616.1736	5.32305	0.000E+00	275.7479	-1.97057	0.000E+00	2		
7	91	318.2128	-1.42376	0.000E+00	385.0068	-2.49001	0.000E+00	2		
7	92									*
7	93	4878.28	-6.3876	0.000E+00	-444.62	-0.7765	0.000E+00	11		*
7	94									*
7	96									*
7	97									*
7	98	206.2641	-2.57259	0.0032526	-371.2031	0.99046	-0.000807	3		*
7	100									*
7	101									*
7	102									*
7	103									*
7	105									*
7	106									*
8	9	-145.2	-0.738	0.000E+00	-666.8	1.918	0.000E+00	2	x	*
8	10									*
8	11	-212.9	0	0.000E+00	-224.4	0	0.000E+00	2	x	*
8	12									*
8	13	-329.3	0	0.000E+00	-80.58	0	0.000E+00	2	x	*
8	14									*
8	16									*
8	17	542	-6.792	1.655E-02	-131.1	-0.9399	4.690E-04	2	x	*
8	18	-4080.8999	12.859	-1.010E-02	-41.594	-3.5887	4.000E-03	2	x	*
8	20	401.88	0	0.000E+00	281.08	0	0.000E+00	2	x	*
8	21									*
8	22									*
8	23									*
8	24	2356	-3.347	0.000E+00	2157	-3.718	0.000E+00	2	x	*
8	25	555.5	0	0.000E+00	1554	0	0.000E+00	2	x	*
8	27									*
8	31	-309	0	0.000E+00	191.7	0	0.000E+00	2	x	*
8	33									*
8	37									*
8	39									*
8	41									*
8	42	391.2	-0.8799	0.000E+00	3630	-6.23	0.000E+00	2	x	*
8	43									*
8	45									*
8	46									*
8	47									*
8	50									*
8	52	4911.3999	9.8501	0.000E+00	2332.5	-4.0832	0.000E+00	2	x	*
8	53									*
8	55									*
8	57									*
8	58									*
8	59									*
8	60									*
8	78									*
8	83									*
8	86									*
8	105									*
8	106									*
9	10	197.6	0	0.000E+00	-93.08	0	0.000E+00	2	x	
9	11	-16.486	-0.2792	0.000E+00	33.415	0.2191	0.000E+00	2	x	
9	12	-83.57	0	0.000E+00	101.3	0	0.000E+00	2	x	
9	13	3645	-26.91	4.757E-02	695.8	-0.9619	-2.462E-03	2	x	
9	15	-47.97	0	0.000E+00	119.5	0	0.000E+00	2	x	

9	16	-389.6	0.1944	1.863E-03	2831	-13.01	1.558E-02	2	x	
9	17	1732	-9.896	1.410E-02	1460	-13.73	2.917E-02	2	x	
9	18	-1908.7	4.1057	0.000E+00	307.16	-0.8161	0.000E+00	2	x	
9	19	-191	0.6835	0.000E+00	79.08	-0.3808	0.000E+00	2	x	
9	20	-109.51	0.9689	0.000E+00	178.22	-0.9168	0.000E+00	2	x	
9	21	-99.976	0	0.000E+00	55.27	0	0.000E+00	2	x	
9	22	-18.695	-0.5261	0.000E+00	-218.94	1.0749	0.000E+00	2	x	
9	23	810.17	-3.2209	2.144E-03	-48.641	-0.795	3.713E-03	2	x	
9	24	-208.71	0.8293	-1.400E-03	155.73	1.4412	-2.500E-03	3	x	
9	25	1297	-1.365	-2.253E-02	1375	2.499	6.309E-03	2	x	
9	26	-35.89	-0.1009	0.000E+00	-32.6	0.0847	0.000E+00	2	x	
9	27	-169.6	2.986	0.000E+00	-328.1	0.3045	0.000E+00	2	x	
9	28	419.9	0.0977	0.000E+00	315.3	-0.5617	0.000E+00	2	x	
9	29	2.714	0	0.000E+00	64.41	0	0.000E+00	2	x	
9	30	-986	3.847	0.000E+00	277	-1.357	0.000E+00	2	x	
9	31	478.5	-1.148	0.000E+00	-72.58	0.4909	0.000E+00	2	x	
9	32	346.6	-0.7017	0.000E+00	-182	0.7905	0.000E+00	2	x	
9	33	-717.76	2.9431	0.000E+00	319.69	-1.4362	0.000E+00	2	x	
9	34	-62.43	-0.8977	0.000E+00	-481.2	9.604	0.000E+00	2	x	
9	35	-76.87	0.5372	0.000E+00	38.06	-0.5189	0.000E+00	2	x	
9	36									*
9	37	64.01	-1.077	0.000E+00	-153.4	3.143	0.000E+00	2	x	
9	38									*
9	39	80.792	-3.702	1.159E-02	1955.5	-10	1.139E-02	2	x	
9	40									*
9	41	64.21	0	0.000E+00	-148.3	0	0.000E+00	2	x	
9	42	437.74	-2.7983	3.640E-03	364.42	2.1022	-4.653E-03	11		
9	43	-62.857	0.2898	0.000E+00	80.038	-0.1012	0.000E+00	2	x	
9	44									*
9	45	-497.98	0.7972	2.982E-04	945.14	-3.8168	4.535E-03	2	x	
9	46									*
9	47	502.1003	0.3401	0.000E+00	141.0113	-0.9829	0.000E+00	4	x	
9	48	37.369	0	0.000E+00	-116.4047	0	0.000E+00	4	x	
9	49	410.65	-1.1056	0.000E+00	-201.11	0.7123	0.000E+00	9		
9	52	-153.7	0.242	0.000E+00	2311.5	-6.6054	0.000E+00	2	x	
9	53									*
9	54									*
9	55									*
9	56									*
9	60									*
9	61									*
9	62									*
9	63									*
9	64									*
9	65									*
9	67									*
9	68									*
9	69									*
9	70									*
9	74									*
9	75									*
9	76									*
9	77									*
9	80									*
9	81									*
9	82									*
9	83									*
9	84	173.4451	-5.52695	0.0160979	958.3726	-4.73012	0.0047161	3		
9	85	824.1235	-2.88368	0.0041569	670.0023	-5.05233	0.0074865	3		
9	86									
9	87	99.5504	0.45575	0.000E+00	-1504.1909	4.63058	0.000E+00	2		
9	88									*
9	89	147.2528	-2.74448	0.000E+00	177.8232	-2.24998	0.000E+00	2		
9	90	331.1518	-1.11421	0.000E+00	-30.955	-0.71244	0.000E+00	2		
9	91	571.6566	-4.43975	0.000E+00	-1449.5725	4.44554	0.000E+00	2		
9	93									*
9	94									*
9	98	519.4855	-5.4673	0.0068391	3306.3645	0.15196	-0.0082641	3		
9	101									*
9	102									*
9	103									*
9	106									*
10	11	-208.4	0	0.000E+00	389.7	0	0.000E+00	2		
10	12	-160.7	0	0.000E+00	226.6	0	0.000E+00	2		
10	13	209	-0.6241	0.000E+00	235.7	0.1314	0.000E+00	2		
10	19									*
10	20	435.64	0	0.000E+00	-188	0	0.000E+00	2		
10	21	985.7	-2.986	0.000E+00	-888.3	3.426	0.000E+00	2		
10	22	-41.537	0	0.000E+00	354.71	0	0.000E+00	3	x	

15	78									*
15	79									*
16	17									*
16	19									*
16	21									*
16	22	-473	0.8883	0.000E+00	406.8	-1.524	0.000E+00	2		
16	24	215.9	-1.399	0.000E+00	-825.9	3.15	0.000E+00	2		
16	25	1622	-4.812	-1.856E-02	-94.87	-9.612	3.722E-02	2	x	
16	28									*
16	31									*
16	38	-7.532	-0.8077	0.000E+00	35.16	0.09723	0.000E+00	2		*
16	39	965	0	0.000E+00	-311.9	0	0.000E+00	2		
16	41									*
16	42	324.15	-1.4264	0.000E+00	-198.32	1.452	0.000E+00	11		
16	43									*
16	44									*
16	45	-420.24	0.2632	0.000E+00	-1035.8	3.078	0.000E+00	2		
16	47	-729.5023	6.2811	0.000E+00	-66.6079	-0.696	0.000E+00	4		
16	48	2111.2449	0	0.000E+00	-235.6095	0	0.000E+00	4		
16	56	2662.02	-13.9855	1.77E-02	-1780.41	5.7197	-1.65E-03	11		
16	60									*
16	78									*
16	79									*
17	18	74.285	14.613	-2.830E-02	-558.39	1.2436	-7.000E-04	2	x	
17	19	393.9	-4.703	9.003E-03	2987	-9.336	7.147E-03	2	x	
17	20									*
17	21	582.1	-2.33	3.770E-04	-338	3.372	-3.676E-03	2	x	
17	24	3986	-16.15	1.635E-02	2626	-10.59	1.466E-02	2	x	
17	25	3709.2	0	0.000E+00	1583.8	0	0.000E+00	2	x	
17	27	3770	1.686	0.000E+00	1.655	-1.164	0.000E+00	2	x	
17	31	1268	-3.042	0.000E+00	-818.8	3.229	0.000E+00	2	x	
17	39	-391.9	0	0.000E+00	650.7	0	0.000E+00	2	x	
17	42	1371	-3.323	0.000E+00	1091	-0.2657	0.000E+00	2	x	
17	43									*
17	45									*
17	46									*
17	47	1271.4183	-6.4373	6.451E-03	-2476.1787	10.9894	-9.617E-03	4		
17	62									*
17	63									*
17	75									*
17	76									*
17	78									*
17	92									*
18	19	746.1208	-2.1937	0.000E+00	-2307.7947	5.8186	0.000E+00	3	x	
18	20	-451.49	-0.4031	0.000E+00	-2617.7	4.614	0.000E+00	3	x	
18	21	-67.106	-0.4933	0.000E+00	-1592.8499	2.8397	0.000E+00	3	x	
18	22	-978.246	2.1884	0.000E+00	946.7893	-4.9886	0.000E+00	3	x	
18	23									*
18	24	229.6591	-1.5005	0.000E+00	-2110.9729	6.3625	0.000E+00	3	x	
18	25									*
18	27									*
18	33	-713.65	1.9191	0.000E+00	-763.19	0.603	0.000E+00	3	x	
18	35									*
18	37									*
18	38	197.9454	-0.3316	-4.000E-04	-1052.5208	1.6854	2.700E-03	3	x	
18	39									*
18	40									*
18	42	268.23	-1.4137	0.000E+00	-5894.1	13.088	0.000E+00	11		
18	43	-250.2521	0.3811	0.000E+00	-1269.7316	2.6335	0.000E+00	3	x	
18	44									*
18	45	-516.3073	1.6943	0.000E+00	-1646.7843	2.7237	0.000E+00	3	x	
18	47	489.9347	-0.5591	-1.020E-03	-2250.6443	5.4638	-1.500E-04	4	x	
18	50									*
18	52	-674.0007	1.8854	0.000E+00	4998.5674	1.1962	0.000E+00	3	x	
18	54									*
18	56									*
18	61									*
18	77									*
18	78									*
18	80									*
18	81									*
18	82									*
18	86									*
18	100									*
19	20									*
19	21	176.5	-1.237	0.000E+00	-368.7	1.992	0.000E+00	2	x	
19	22	-78.96	0	0.000E+00	14.76	0	0.000E+00	2		
19	23									*
19	24	65.82	-0.6265	0.000E+00	357.6	0.7676	0.000E+00	2		
19	25	1283	3.361	-2.988E-02	2331	-9.238	1.158E-02	2	x	

