Supplementary Material

A.1. Joback and Reid, 1987

Table A 1 – Joback and Reid group contributions for the estimation of the components properties [148].

Group	T_{b_i}	T_{C_i}	P_{C_i}	V_{C_i}	T_{m_i}	ΔH_{vap_i}	ΔH_{fus_i}
$-\mathrm{CH_3}$	23.58	0.0141	-0.0012	65	-5.1	2.373	0.908
$-\mathrm{CH_2}-$	22.88	0.0189	0	56	11,27	2.226	2.590
$=\mathrm{CH}-$	26.73	0.0129	-0.0006	46	8.73	1.691	0.749
$-\mathrm{COOH}$	169.09	0.0791	0.0077	89	155.5	0.636	−1.460

Table A 1 (continued) – Joback and Reid group contributions for the estimation of the components properties [148].

Group	C_{p,a_i}	C_{p,b_i}	C_{p,c_i}	C_{p,d_i}	v_{A_i}	v_{B_i}
$-\mathrm{CH_3}$	1.95E+01	-8.08E-03	1.53E-04	-9.67E-08	548.29	-1.719
$-\mathrm{CH_2}-$	-9.09E-01	9.50E-02	-5.44E-05	1.19E-08	94.16	-0.199
$=\mathrm{CH}-$	-8.00	1.05E-01	-9.63E-05	3.56E-08	82.28	-0.242
$-\mathrm{COOH}$	2.41E+01	4.27E-02	8.04E-05	-6.87E-08	1317.23	-2.578

A.2. Constantinou and Gani, 1994

Table A 2 – Constantinou and Gani group contributions for the estimation of the components properties – first order [149], [162]

Group	t_{b1i}	t_{c1k}	P_{c1k} $(\mathrm{bar}^{-0.5})$	v_{c1k} $(\mathrm{m}^3/\mathrm{kmol})$	t_{m1i}	h_{v1i}	ω_{1i}
$\mathrm{CH_3}$	0.8894	1.6781	0.019904	0.07504	0.4640	4.116	0.296
$\mathrm{CH_2}$	0.9225	3.4920	0.010558	0.05576	0.9246	4.650	0.147
$\mathrm{CH}=\mathrm{CH}$	1.8433	7.3691	0.017865	0.09541	0.3557	2.771	0.252
COOH	5.8337	23.7593	0.011507	0.10188	11.5630	1.284	1.670

Table A 3 – Constantinou and Gani group contributions for the estimation of the components properties – second order [149], [162]

Group	t_{b2j}	t_{c2j}	P_{c2j} $(\mathrm{bar}^{-0.5})$	v_{c2k} $(\mathrm{m}^3/\mathrm{kmol})$	t_{m2j}	h_{v2j}	ω_{2j}
$\mathrm{CH_2}-\mathrm{CH_m}=\mathrm{CH_n}$ $\mathrm{m,n}\ \epsilon(0,2)$	- 0.1406	- 0.5231	0.003538	0.00281	-0.5870	-0.369	-0.012

A.3. Marrero-Marejón and Pardillo-Fontdevila, 1999

Table A 4 – Marrero-Marejón and Pardillo-Fontdevila method group-interaction contributions to determine pure compounds properties [150]

Interactions with	t_{bbk}	t_{cbk}	p_{cbk}	v_{cbk}
$CH_3 -$ and $- CH_2 -$	194.25	-0.0227	-0.0430	88.6
$-CH_2 -$ and $- CH_2 -$	244.88	-0.0206	-0.0272	56.6
$-CH_2 -$ and $= CH -$	201.80	0.8636	0.0818	50.7
$-CH_2 -$ and $- COOH$	1180.39	-0.0932	-0.0253	114.0
$= CH -$ and $= CH -$	334.64	-1.7660	-0.2291	47.8

A.4. Marrero and Gani, 2001

Table A 5 – Marrero and Gani group contributions for the estimation of the components properties – first order [151]

Group	t_{b1i}	t_{c1k}	P_{c1k}	V_{c1i}	t_{m1i}	H_{v1i}	H_{fus1i}
CH_3	0.8491	1.7506	0.018615	68.35	0.6953	0.217	1.660
CH_2	0.7141	1.3327	0.013547	56.28	0.2515	4.910	2.639
$CH = CH$	1.5597	3.0741	0.023003	98.43	-0.3730	9.456	4.441
$COOH$	5.1108	14.6038	0.009885	90.66	0.0256	17.002	10.692

Table A 6 – Marrero and Gani group contributions for the estimation of the components properties – second order [151]

Group	t_{b2j}	t_{c2j}	P_{c2j}	V_{c2j}	t_{m2j}	H_{v2j}	H_{fus2j}
$CH_2 - CH_m = CH_n$ $m, n \epsilon (0,2)$	-0.0537	0.0262	0.000815	0.14	-0.1077	-0.060	-0.632

A.5. Nannoolal et al., 2004

Table A 7 – Nannoolal et al. group contributions for the estimation of the components properties [152], [156]

Group	T_b	$T_C \times 10^3$	$P_C \times 10^4$	V_C
$-CH_3$	177.3066	41.8682	8.1620	28.7855
$-CH_2 -$	239.4531	40.0977	5.2623	32.0493
$-COOH$	1080.3139	199.9042	3.9873	40.3909
$> C = C <$	412.6276	45.4406	9.6413	48.1957

A.6. Wilson and Jasperson, 1996

Table A 8 – Wilson and Jasperson for the estimation of the component's properties [155]

Group	t_{cJ}	p_{cJ}
H	0.002793	0.126600
C	0.008532	0.729830
O	0.020341	0.433600
$COOH$	0.017	0.5

A.7. WAGNER25. Liquid vapour pressure

Table A 9 – WAGNER25. TDE Wagner 25 liquid vapour pressure (N/m^2)

	CN	$C_1\ (-)$	$C_2\ (-)$	$C_3\ (-)$	$C_4\ (-)$	$C_5\ (\ln(\mathrm{P_C}))(-)$	$C_6.T_c(K)$	$T_{lower}\ (K)$	$T_{upper}\ (K)$
CN:0	C8:0	-14.5947	16.4471	-24.9002	13.0849	14.8654	693.71	289.656	693.71
	C10:0	-9.55395	4.25681	-13.2861	1.10672	14.54584	723.769	304.543	723.769
	C12:0	-15.1121	16.9579	-26.4645	9.59019	14.4736	743	316.969	743
	C14:0	-15.4539	16.8372	-25.7647	5.48625	14.30994	763	327.306	763
	C16:0	-8.81196	-2.08817	-2.79714	-20.984	14.21405	785	335.642	785
	C 18:0	-10.5921	2.53244	-9.70946	-12.4752	14.10047	803	342.624	803
	C 20:0	-13.2693	7.32725	-14.9518	-2.90727	13.99791	820	348.211	820
	C 22:0	-13.9916	9.16511	-18.5369	2.20194	13.91998	837	353.78	837
	C 24:0	-10.4801	3.78806	-7.79263	-4.98268	13.65123	825	355.6	825
CN:1	C16:1	-12.2223	5.37393	-11.5532	-5.34164	14.21261	789	274.8	789
	C18:1	-12.2064	5.35822	-11.517	-5.34069	14.02856	796	286.57	796
	C20:1	-	-	-	-	-	-	-	-
	C22:1	-12.1692	5.32145	-11.4321	-5.33829	13.79869	806	306.13	806
	C24:1	-	-	-	-	-	-	-	-
CN:2	C18:2	-11.6351	4.80818	-10.2366	-5.27866	14.25142	787	267.6	787
CN:3	C18:3	-11.7961	4.9602	-10.5927	-5.30154	14.13086	777	260	777