

PURE COMPONENT PARAMETERS :

COMPONENT (I)		V(I) (ML/MOL)	R(I)	Q(I)
DEUTERIUM OXIDE	D2O	18.13	.9200	1.4000
HYDROGEN CHLORIDE	HCL	29.52	0.0000	0.0000
HYDROGEN FLUORIDE	HF	20.19	.6038	.7480
HYDROGEN IODIDE	HI	45.63	0.0000	0.0000
NITRIC ACID	HNO3	41.93	1.6375	1.6040
HYDROGEN PEROXIDE	H2O2	23.58	1.7400	1.7400
AMMONIA	H3N	26.65	0.0000	0.0000
HYDRAZINE	H4N2	31.85	1.3896	1.3920
HYDROGEN CYANIDE	CHN	39.31	1.1957	1.1840
FORMALDEHYDE	CH2O	36.83	1.2248	1.2560
FORMIC ACID	CH2O2	37.91	1.5280	1.5320
O-DEUTEROMETHANOL	CH3DO	40.67	1.4311	1.4320
NITROMETHANE	CH3NO2	53.96	2.0086	1.8680
METHANOL	CH4O	40.73	1.4311	1.4320
ACETONITRILE	C2H3N	52.86	1.8701	1.7240
ACETALDEHYDE	C2H4O	56.62	1.8991	1.7960
ETHYLENE OXIDE	C2H4O	49.92	1.5927	1.3200
ACETIC ACID	C2H4O2	57.54	2.2024	2.0720
O-DEUTEROETHANOL	C2H5DO	58.12	2.1055	1.9720
ETHANOL	C2H6O	58.69	2.1055	1.9720
DIMETHYLSULFOXIDE	C2H6OS	71.30	2.8266	2.4720
1,2-ETHANEDIOL	C2H6O2	55.92	2.4088	2.2480
ETHYLAMINE	C2H7N	67.81	2.2703	2.0840
ETHANOLAMINE	C2H7NO	60.41	2.5736	2.3600
ETHYLENEDIAMINE	C2H8N2	67.83	2.7384	2.4720
ACROLEIN	C3H4O	66.84	2.3434	2.1240

COMPONENT (I)		V(I) (ML/MOL)	R(I)	Q(I)
ACRYLIC ACID	C3H4O2	68.56	2.6467	2.4000
3-CHLORO-1-PROPENE	C3H5CL	81.62	2.8108	2.4400
ACETONE	C3H6O	74.04	2.5735	2.3360
ALLYL ALCOHOL	C3H6O	68.62	2.5498	2.3000
PROPIONIC ALDEHYDE	C3H6O	73.41	2.5735	2.3360
ETHYL FORMATE	C3H6O2	80.88	2.8042	2.5760
METHYL ACETATE	C3H6O2	79.84	2.8042	2.5760
1,3,5-TRIOXANE	C3H6O3	76.99	2.7549	2.3400
N,N-DIMETHYLFORMAMIDE	C3H7NO	77.44	3.0856	2.7360
N-METHYLACETAMIDE	C3H7NO	76.96	3.1061	2.7320
2-PROPANOL	C3H8O	76.92	2.7791	2.5080
1,2-PROPANEDIOL	C3H8O2	73.68	3.2824	2.7840
GLYCEROL	C3H8O3	73.20	3.5857	3.0600
ISOPROPYLAMINE	C3H9N	86.66	2.9439	2.6200
PROPYLAMINE	C3H9N	83.01	2.9447	2.6240
3-AMINO-1-PROPANOL	C3H9NO	76.46	3.2480	2.9000
ALLYLCYANIDE	C4H5N	80.55	2.9888	2.5920
CROTONITRILE (CIS)	C4H5N	81.58	2.9868	2.5910
CROTONITRILE (TRANS)	C4H5N	81.43	2.9868	2.5910
CROTON ALDEHYDE	C4H6O	82.89	3.0158	2.6630
METHACRYLIC ACID	C4H6O2	84.79	3.3197	3.0600
VINYL ACETATE	C4H6O2	93.10	3.2485	2.9040
ACETIC ANHYDRIDE	C4H6O3	94.96	3.5755	3.2160
PROPYLENE CARBONATE	C4H6O3	85.29	3.2815	2.7360
2-BUTANONE	C4H8O	90.17	3.2479	2.8760
BUTYRALDEHYDE	C4H8O	88.27	3.2479	2.8760

COMPONENT (I)		V(I) (ML/MOL)	R(I)	Q(I)
ISOBUTYR ALDEHYDE	C4H8O	91.39	3.2471	2.8720
TETRAHYDROFURAN	C4H8O	81.55	2.9415	2.7200
1,4-DIOXANE	C4H8O2	85.71	3.1854	2.6400
ETHYL ACETATE	C4H8O2	98.49	3.4786	3.1160
METHYL PROPIONATE	C4H8O2	96.28	3.4786	3.1160
MORPHOLINE	C4H9NO	87.51	3.4740	2.7960
N,N-DIMETHYLACETAMIDE	C4H9NO	93.02	3.5332	2.9680
1-BUTANOL	C4H10O	91.96	3.4543	3.0520
2-BUTANOL	C4H10O	92.35	3.4535	3.0480
DIETHYL ETHER	C4H10O	104.75	3.3949	3.0160
2-METHYL-1-PROPANOL	C4H10O	92.91	3.4535	3.0480
TERT-BUTANOL	C4H10O	94.88	3.4528	3.1280
1,4-BUTANEDIOL	C4H10O2	88.35	3.7576	3.3280
2,3-BUTANEDIOL	C4H10O2	87.84	3.7560	3.3200
1,1-DIMETHOXYETHANE	C4H10O2	105.82	3.6380	3.2520
2-ETHOXYETHANOL	C4H10O2	96.93	3.6982	3.2920
DIETHYLENE GLYCOL	C4H10O3	94.78	4.0013	3.5680
2-DIMETHYLAMINO ETHANOL	C4H11NO	100.54	3.9664	3.4520
FURFURAL	C5H4O2	83.23	3.1680	2.4840
PYRIDINE	C5H5N	80.86	2.9993	2.1130
FURFURYL ALCOHOL	C5H6O2	87.11	3.3744	2.6600
N-METHYLPYRROLIDONE(2)	C5H9NO	96.44	3.9810	3.2000
3-METHYL-3-BUTEN-1-OL	C5H10O	101.22	3.8972	3.5000
3-METHYLBUTYRALDEHYDE	C5H10O	109.79	0.0000	0.0000
VALERALDEHYDE	C5H10O	106.41	3.9223	3.4160
2-(HYDROXYMETHYL)-TETRAHYDROFURAN	C5H10O2	97.53	3.9184	3.2120

COMPONENT (I)		V(I) (ML/MOL)	R(I)	Q(I)
PROPYL ACETATE	C5H10O2	115.66	4.1530	3.6560
VALERIC ACID	C5H10O2	108.76	4.2256	3.6920
PIPERIDINE	C5H11N	98.94	3.9046	3.0960
3-METHYL-1-BUTANOL	C5H12O	109.22	4.1279	3.5880
1-PENTANOL	C5H12O	108.63	4.1287	3.5920
2-PENTANOL	C5H12O	108.83	4.1279	3.5880
O-DICHLOROBENZENE	C6H4CL2	112.67	4.4376	3.2880
BENZENE	C6H6	89.41	3.1878	2.4000
M-CHLOROANILINE	C6H6CLN	104.90	4.3414	3.2600
PHENOL	C6H6O	83.14	3.5517	2.6800
ANILINE	C6H7N	91.53	3.7165	2.8160
2-METHYLPYRIDINE	C6H7N	99.03	3.7343	2.6810
3-METHYLPYRIDINE	C6H7N	97.88	3.7343	2.6810
4-METHYLPYRIDINE	C6H7N	98.01	3.7343	2.6810
CYCLOHEXANONE	C6H10O	104.18	4.1433	3.3400
METHYLDIHYDROPYRAN	C6H10O	107.47	3.0711	2.3840
6-CAFROLACTAM	C6H11NO	110.94	4.6106	3.7240
NITRO CYCLOHEXANE	C6H11NO2	121.73	4.9264	3.9480
CYCLOHEXANE	C6H12	108.75	4.0464	3.2400
1-HEXENE	C6H12	125.89	4.2697	3.6440
4-METHYL-2-PENTANONE	C6H12O	125.81	4.5959	3.9520
BUTYL ACETATE	C6H12O2	132.54	4.8274	4.1960
4,4-DIMETHYL-1,3-DIOXANE	C6H12O2	120.60	4.5327	3.7960
PROPYL PROPIONATE	C6H12O2	131.85	4.8274	4.1960
2-METHYLPYPERIDINE	C6H13N	117.57	4.5782	3.6320
HEXANE	C6H14	131.61	4.4998	3.8560

COMPONENT (I)		V(I) (ML/MOL)	R(I)	Q(I)
1-HEXANOL	C6H14O	125.24	4.8031	4.1320
4-METHYL-2-PENTANOL	C6H14O	127.33	4.8015	4.1240
TRIETHYLAMINE	C6H15N	139.96	5.0118	4.2560
2,6-DIMETHYLPYRIDINE	C7H9N	116.48	4.4693	3.2490
DIETHYL MALONATE	C7H12O4	151.81	0.0000	0.0000
1-HEPTENE	C7H14	140.27	4.9441	4.1840
BUTYL PROPIONATE	C7H14O2	148.72	5.5018	4.7360
ISOPENTYL ACETATE	C7H14O2	150.27	5.5010	4.7320
BUTYL BUTYRATE	C8H16O2	165.60	6.1762	5.2760
OCTANOIC ACID	C8H16O2	159.08	6.2488	5.3120
OCTANE	C8H18	163.54	5.8486	4.9360
2-ETHYL-1-HEXANOL	C8H18O	156.38	6.1511	5.2080
1-OCTANOL	C8H18O	158.41	6.1519	5.2120
BENZYL ACETATE	C9H10O2	142.82	5.5992	4.3880
ISOPROPYLBENZENE	C9H12	140.17	5.2708	4.0440
NICOTINE	C10H14N2	160.73	6.4898	4.6210
DECANE	C10H22	195.94	7.1974	6.0160