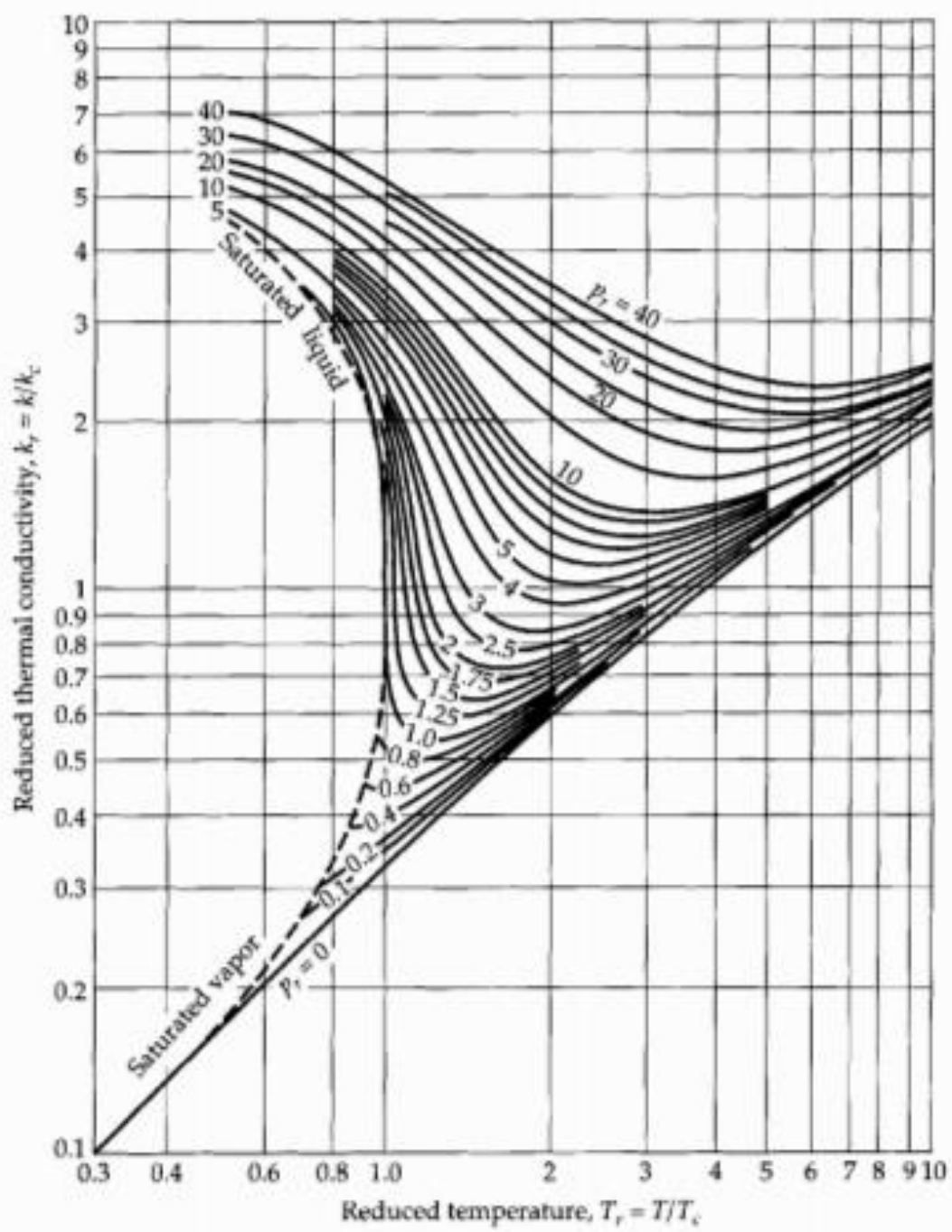
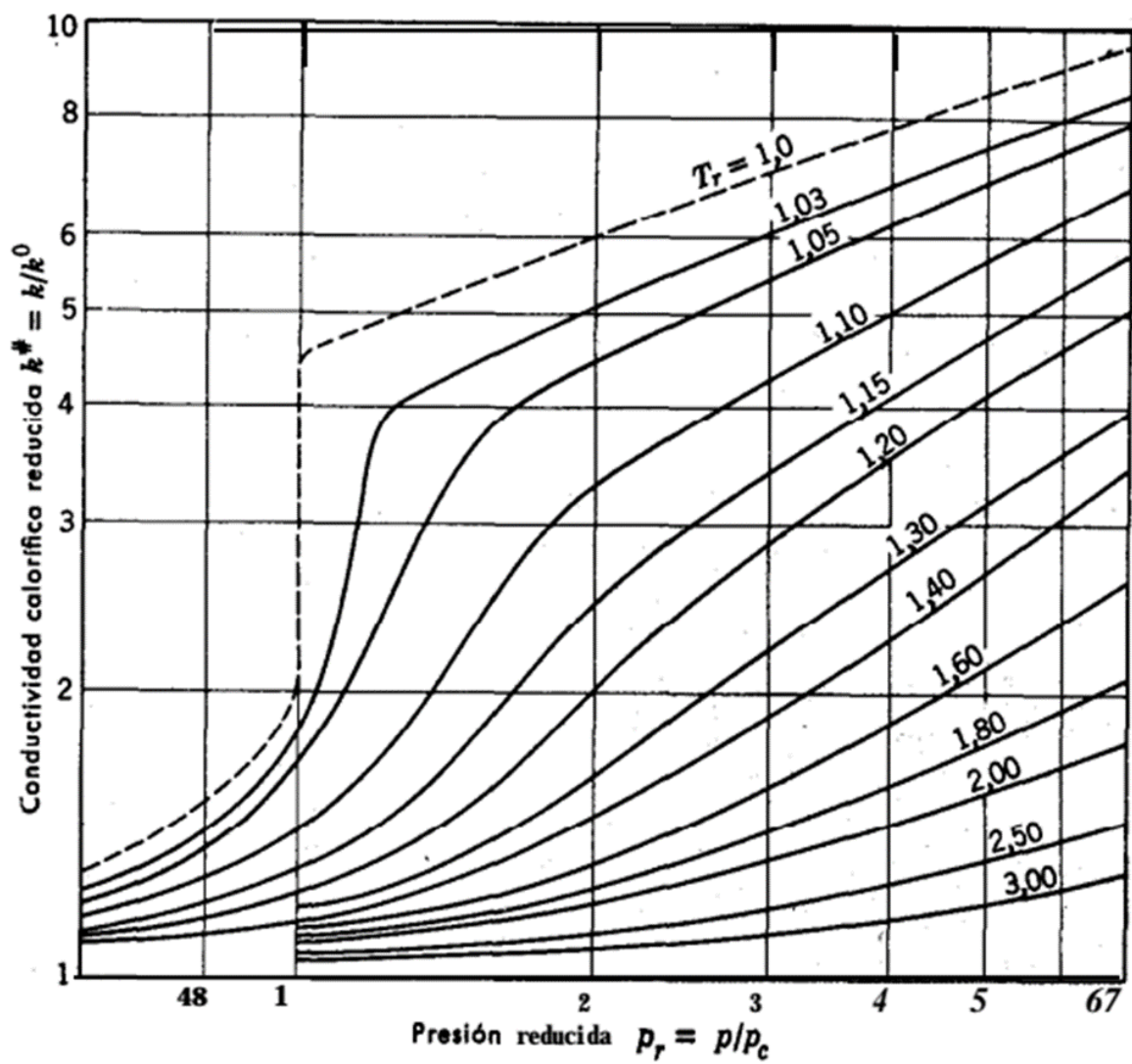


Table E.1 Lennard-Jones (6–12) Potential Parameters and Critical Properties

		Lennard-Jones parameters			Critical properties ^{a,b}				
Substance	Molecular Weight <i>M</i>	σ (Å)	ϵ/κ (K)	Ref.	<i>T_c</i> (K)	<i>p_c</i> (atm)	\tilde{V}_c (cm ³ /g-mole)	μ_c (g/cm ³ · s × 10 ⁶)	<i>k_c</i> (cal/cm ³ · s · K)
Light elements:									
H ₂	2.016	2.915	38.0	<i>a</i>	33.3	12.80	65.0	34.7	—
He	4.003	2.576	10.2	<i>a</i>	5.26	2.26	57.8	25.4	—
Noble gases:									
Ne	20.180	2.789	35.7	<i>a</i>	44.5	26.9	41.7	156.	79.2
Ar	39.948	3.432	122.4	<i>b</i>	150.7	48.0	75.2	264.	71.0
Kr	83.80	3.675	170.0	<i>b</i>	209.4	54.3	92.2	396.	49.4
Xe	131.29	4.009	234.7	<i>b</i>	289.8	58.0	118.8	490.	40.2
Simple polyatomic gases:									
Air	28.964 ⁱ	3.617	97.0	<i>a</i>	132.4 ⁱ	37.0 ^j	86.7 ⁱ	193.	90.8
N ₂	28.013	3.667	99.8	<i>b</i>	126.2	33.5	90.1	180.	86.8
O ₂	31.999	3.433	113.	<i>a</i>	154.4	49.7	74.4	250.	105.3
CO	28.010	3.590	110.	<i>a</i>	132.9	34.5	93.1	190.	86.5
CO ₂	44.010	3.996	190.	<i>a</i>	304.2	72.8	94.1	343.	122.
NO	30.006	3.470	119.	<i>a</i>	180.	64.	57.	258.	118.2
N ₂ O	44.012	3.879	220.	<i>a</i>	309.7	71.7	96.3	332.	131.
SO ₂	64.065	4.026	363.	<i>c</i>	430.7	77.8	122.	411.	98.6
F ₂	37.997	3.653	112.	<i>a</i>	—	—	—	—	—
Cl ₂	70.905	4.115	357.	<i>a</i>	417.	76.1	124.	420.	97.0
Br ₂	159.808	4.268	520.	<i>a</i>	584.	102.	144.	—	—
I ₂	253.809	4.982	550.	<i>a</i>	800.	—	—	—	—
Hydrocarbons:									
CH ₄	16.04	3.780	154.	<i>b</i>	191.1	45.8	98.7	159.	158.
CH≡CH	26.04	4.114	212.	<i>d</i>	308.7	61.6	112.9	237.	—
CH ₂ =CH ₂	28.05	4.228	216.	<i>b</i>	282.4	50.0	124.	215.	—
C ₂ H ₆	30.07	4.388	232.	<i>b</i>	305.4	48.2	148.	210.	203.
CH ₃ C≡CH	40.06	4.742	261.	<i>d</i>	394.8	—	—	—	—
CH ₃ CH=CH ₂	42.08	4.766	275.	<i>b</i>	365.0	45.5	181.	233.	—
C ₃ H ₈	44.10	4.934	273.	<i>b</i>	369.8	41.9	200.	228.	—
<i>n</i> -C ₄ H ₁₀	58.12	5.604	304.	<i>b</i>	425.2	37.5	255.	239.	—
<i>i</i> -C ₄ H ₁₀	58.12	5.393	295.	<i>b</i>	408.1	36.0	263.	239.	—
<i>n</i> -C ₅ H ₁₂	72.15	5.850	326.	<i>b</i>	469.5	33.2	311.	238.	—
<i>i</i> -C ₅ H ₁₂	72.15	5.812	327.	<i>b</i>	460.4	33.7	306.	—	—
C(CH ₃) ₄	72.15	5.759	312.	<i>b</i>	433.8	31.6	303.	—	—
<i>n</i> -C ₆ H ₁₄	86.18	6.264	342.	<i>b</i>	507.3	29.7	370.	248.	—
<i>n</i> -C ₇ H ₁₆	100.20	6.663	352.	<i>b</i>	540.1	27.0	432.	254.	—
<i>n</i> -C ₈ H ₁₈	114.23	7.035	361.	<i>b</i>	568.7	24.5	492.	259.	—
<i>n</i> -C ₉ H ₂₀	128.26	7.463	351.	<i>b</i>	594.6	22.6	548.	265.	—
Cyclohexane	84.16	6.143	313.	<i>d</i>	553.	40.0	308.	284.	—
Benzene	78.11	5.443	387.	<i>b</i>	562.6	48.6	260.	312.	—
Other organic compounds:									
CH ₄	16.04	3.780	154.	<i>b</i>	191.1	45.8	98.7	159.	158.
CH ₃ Cl	50.49	4.151	355.	<i>c</i>	416.3	65.9	143.	338.	—
CH ₂ Cl ₂	84.93	4.748	398.	<i>c</i>	510.	60.	—	—	—
CHCl ₃	119.38	5.389	340.	<i>e</i>	536.6	54.	240.	410.	—
CCl ₄	153.82	5.947	323.	<i>e</i>	556.4	45.0	276.	413.	—
C ₂ N ₂	52.034	4.361	349.	<i>e</i>	400.	59.	—	—	—
COS	60.076	4.130	336.	<i>e</i>	378.	61.	—	—	—
CS ₂	76.143	4.483	467.	<i>e</i>	552.	78.	170.	404.	—
CCl ₂ F ₂	120.91	5.116	280.	<i>b</i>	384.7	39.6	218.	—	—





$\kappa T/\varepsilon$ or $\kappa T/\varepsilon_{AB}$	$\Omega_\mu = \Omega_k$ (for viscosity and thermal conductivity)	$\Omega_{T,AB}$ (for diffusivity)	$\kappa T/\varepsilon$ or $\kappa T/\varepsilon_{AB}$	$\Omega_\mu = \Omega_k$ (for viscosity and thermal conductivity)	$\Omega_{T,AB}$ (for diffusivity)
0.30	2.840	2.649	2.7	1.0691	0.9782
0.35	2.676	2.468	2.8	1.0583	0.9682
0.40	2.531	2.314	2.9	1.0482	0.9588
0.45	2.401	2.182	3.0	1.0388	0.9500
0.50	2.284	2.066	3.1	1.0300	0.9418
0.55	2.178	1.965	3.2	1.0217	0.9340
0.60	2.084	1.877	3.3	1.0139	0.9267
0.65	1.999	1.799	3.4	1.0066	0.9197
0.70	1.922	1.729	3.5	0.9996	0.9131
0.75	1.853	1.667	3.6	0.9931	0.9068
0.80	1.790	1.612	3.7	0.9868	0.9008
0.85	1.734	1.562	3.8	0.9809	0.8952
0.90	1.682	1.517	3.9	0.9753	0.8897
0.95	1.636	1.477	4.0	0.9699	0.8845
1.00	1.593	1.440	4.1	0.9647	0.8796
1.05	1.554	1.406	4.2	0.9598	0.8748
1.10	1.518	1.375	4.3	0.9551	0.8703
1.15	1.485	1.347	4.4	0.9506	0.8659
1.20	1.455	1.320	4.5	0.9462	0.8617
1.25	1.427	1.296	4.6	0.9420	0.8576
1.30	1.401	1.274	4.7	0.9380	0.8537
1.35	1.377	1.253	4.8	0.9341	0.8499
1.40	1.355	1.234	4.9	0.9304	0.8463
1.45	1.334	1.216	5.0	0.9268	0.8428
1.50	1.315	1.199	6.0	0.8962	0.8129
1.55	1.297	1.183	7.0	0.8727	0.7898
1.60	1.280	1.168	8.0	0.8538	0.7711
1.65	1.264	1.154	9.0	0.8380	0.7555
1.70	1.249	1.141	10.0	0.8244	0.7422
1.75	1.235	1.128	12.0	0.8018	0.7202
1.80	1.222	1.117	14.0	0.7836	0.7025
1.85	1.209	1.105	16.0	0.7683	0.6878
1.90	1.198	1.095	18.0	0.7552	0.6751
1.95	1.186	1.085	20.0	0.7436	0.6640
2.00	1.176	1.075	25.0	0.7198	0.6414
2.10	1.156	1.058	30.0	0.7010	0.6235
2.20	1.138	1.042	35.0	0.6854	0.6088
2.30	1.122	1.027	40.0	0.6723	0.5964
2.40	1.107	1.013	50.0	0.6510	0.5763
2.50	1.0933	1.0006	75.0	0.6140	0.5415
2.60	1.0807	0.9890	100.0	0.5887	0.5180