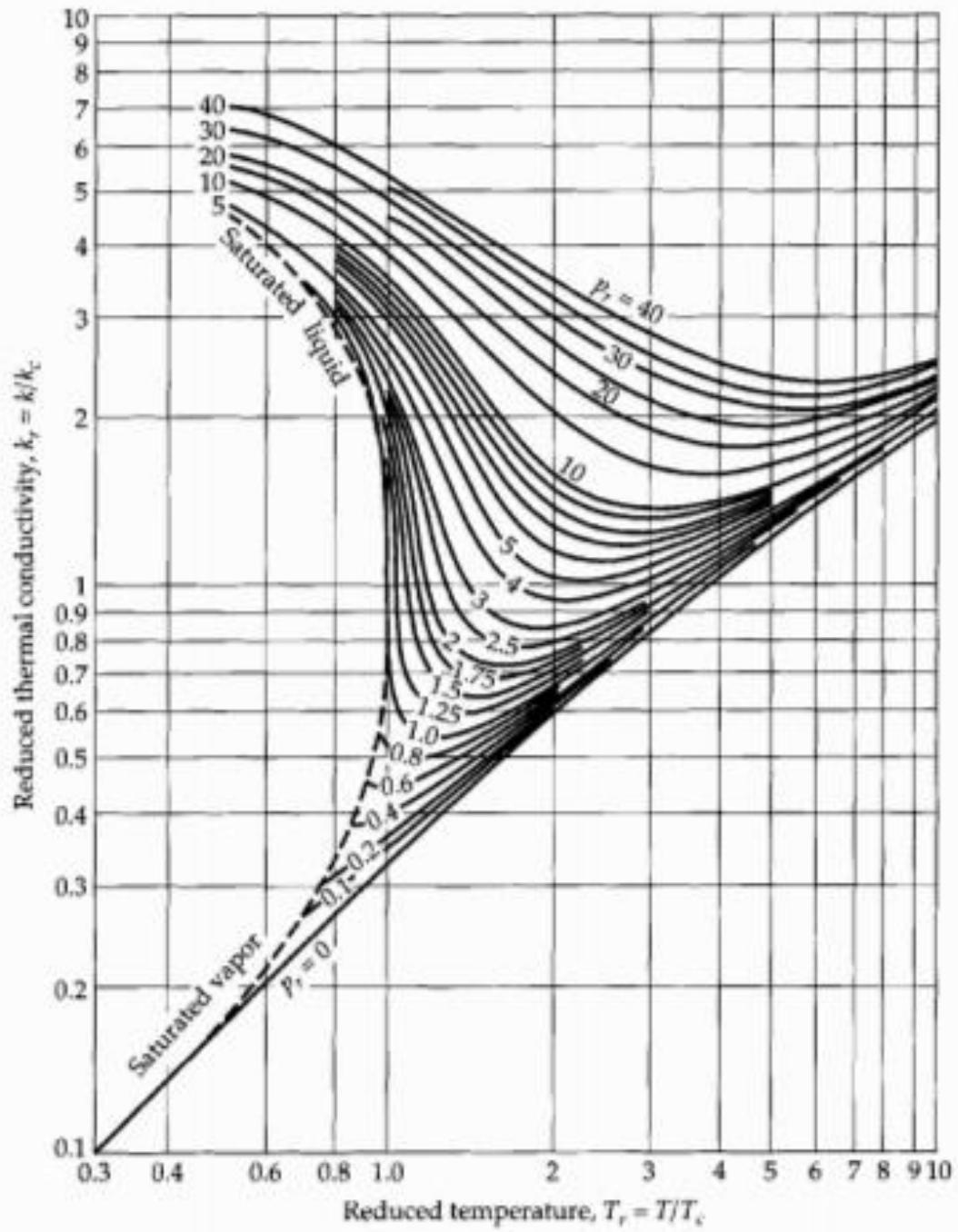
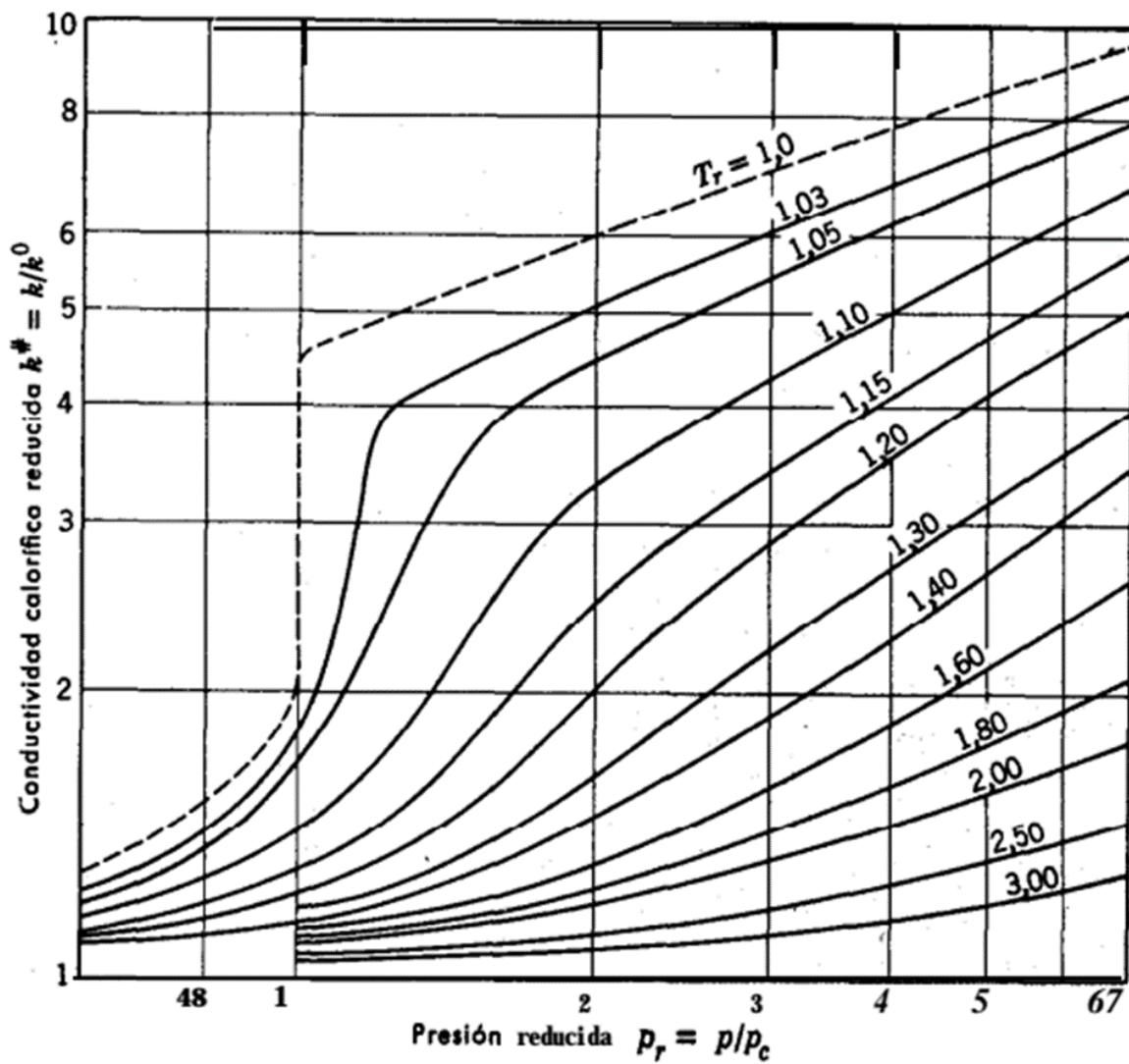


**Table E.1** Lennard-Jones (6–12) Potential Parameters and Critical Properties

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





| $\kappa T/\epsilon$<br>or<br>$\kappa T/\epsilon_{AB}$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_{D,AB}$<br>(for<br>diffusivity) | $\kappa T/\epsilon$<br>or<br>$\kappa T/\epsilon_{AB}$ | $\Omega_\mu = \Omega_k$<br>(for viscosity<br>and thermal<br>conductivity) | $\Omega_{D,AB}$<br>(for<br>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                                  |