

One-Component Classical Monatomic Gas by James Pate Williams, Jr.

Reference: **An Introduction to Statistical Thermodynamics** (c) 1960 by Terrell L. Hill
Chapter 15-2

We use the Lennard-Jones Potential to compute the second virial coefficient of a one-component classical monatomic gas using the integral equation:

$$B_2(T) = -2\pi r^{*3} \int_0^{\infty} \left[\left(e^{-2\epsilon/kT} y^{-6} - \frac{\epsilon}{kT} y^{-12} \right) - 1 \right] y^2 dy$$

Where:

$$y = \frac{r}{r^*}$$

The integral was evaluated using Simpson's Rule. The number of steps was 25,000 and the integral was calculated for upper bounds of 25, 50, and 75.

kT/e	Integral 1	Integral 2	Integral 3
1	-3.7606257341	-3.7608603064	-3.7608838877
2	-0.9314489152	-0.9315662013	-0.9315779920
3	-0.1726620382	-0.1727402289	-0.1727480894
4	0.16890058306	0.16884194000	0.16883604466
5	0.35834145361	0.35829453916	0.35828982289
6	0.47615906135	0.47611996598	0.47611603575
7	0.55491624704	0.55488273672	0.55487936796
8	0.61021866847	0.61018934694	0.61018639927
9	0.65044359689	0.65041753330	0.65041491316
10	0.68047072517	0.68044726795	0.68044490981
11	0.70332357454	0.70330224979	0.70330010603
12	0.72096852444	0.72094897675	0.72094701164
13	0.73473530966	0.73471726564	0.73471545169
14	0.74555248264	0.74553572748	0.74553404310
15	0.75408611848	0.75407048033	0.75406890824
16	0.76082504581	0.76081038504	0.76080891121
17	0.76613512423	0.76612132586	0.76611993872
18	0.77029488546	0.77028185367	0.77028054360
19	0.77351956773	0.77350722182	0.77350598070
20	0.77597770498	0.77596597637	0.77596479730
21	0.77780281533	0.77779164522	0.77779052230
22	0.77910178859	0.77909112622	0.77909005434
23	0.77996100466	0.77995080587	0.77994978060
24	0.78045086295	0.78044108911	0.78044010655
25	0.78062918073	0.78061979784	0.78061885459

C:\Users\James\OneDrive\LennardJonesB2\x64\Debug\LennardJonesB2.exe (process 436) exited with code 0 (0x0).
Press any key to close this window . . .
As is readily apparent, the integral slowly converges.

