|  |  |  |  |
| --- | --- | --- | --- |
| Temp | NPT Volume | NPT Enthalpy | NVT Energy |
| 350 | 68527.23 | -12898.49 | -12902.83 |
| 300 | 68193.84 | -12951.55 | -12954.15 |
| 250 | 67862.53 | -12999.80 | -13003.99 |
|  |  |  |  |
| \*K Aluminum (Gpa) | \*K Aluminum (eV/A^3) |  |  |
| 72.20 | 4.51E-01 |  |  |
|  |  |  |  |
| α = 1/V(dV/dT)P | Cp = (dH/dT) | Cv = Cp - α^2(KVT) | Cv = (dE/dT)V |
| 9.75E-05 (1/K) | 1.013 (eV/K) | 0.926 (eV/K) | 1.012 (eV/K) |

\*Literature values were used for Isothermal Bulk Modulus (K)