

Peachtree 2012 Serial Number

Thermodynamics State Value for Lennard-Jones Fluid

Non-Dimensional Temperature $T^* =$ $T^* = kT/\epsilon$ Iso_T

Non-dimensional number density $\rho^* =$ $\rho^* = \rho \sigma^3 = (N/V) \sigma^3$ Iso_Rho

Calculator EXIT

Rea Nicolas et al

$\rho^* = \rho \sigma^3 / \epsilon$ Pressure

$P / (\rho kT)$

$A_e^* = A_e / (N\epsilon)$ Excess Helmholtz Free Energy / atom
 $A_e = A - A_{ideal gas}$

$A_e / (NkT)$

$\mu_e^* = \mu_e / \epsilon$ Excess Gibbs Free Energy / atom
 $\mu_e = \mu - \mu_{ideal gas}$

$\mu_e / (kT)$

$U^* = U / (N\epsilon)$ Configurational Internal Energy / atom
 $U / (NkT)$ Total Potential Energy / atom
Note: $U_e = U$, because $U = 0$ for ideal gas

$E_k = E / (N\epsilon)$ Internal Energy / atom
 $E / (NkT)$ Total Energy / atom

$S_e / (Nk)$ Residual Entropy / atom

$\rho^* =$ Iso_P

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