

## 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

Ree Nicolas et al

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

$P / (\rho kT)$

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

$A^* / (NkT)$

$\mu^* = \mu^* / \epsilon$    Excess Gibbs Free Energy / atom  
 $\mu^* = \mu^* / (kT)$    = Excess Chemical Potential

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

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

$S^* / (Nk)$    Residual Entropy / atom

$\rho^* =$   Iso\_P

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