1. Theory for Heat of Vaporization

I) Vetere Method (HC_HVPVET)

Vetere proposed a following expression for heat of vaporization at normal boiling point.

$$\Delta H_{vb} = RT_b \frac{(1-T_{br})^{0.38}\left(\ln P_c - 0.513 + 0.5066 / \left(P_c T_{br}^2\right)\right)}{1-T_{br} + F\left(1-\left(1-T_{br}\right)^{0.38}\right)\ln T_{br}} \quad (1)$$

F is 1.05 for C_2+ alcohols and dimerizing compounds such as SO_3, NO, and NO_2. Except for such a case, F is 1.0.

For describing the variation of heat of vaporization we use the Watson relation.

$$\Delta H_{vp} = \Delta H_{vb}\left(\frac{1-T_r}{1-T_{br}}\right)^{0.38} \quad (2)$$

Reference

A. Vetere, *Fluid Phase Equilib.*, **106**, 1 (1995)

R.E. Thek and L.I. Stiel, *AIChE J.*, **12**, 599 (1966)

Poling et al., "Properties of Gases and Liquids", 5th ed. McGraw-Hill, New York (2000)

2. KDB Routines for Heat of Vaporization

KDB heat of vaporization calculation subroutine contain a estimation method, which is Vetere method.

Subroutine Name	Description	Required Common Blocks
HC_HVPVET	Vetere Method	HC_NAME, HC_PROP

I) HC_HVPVET

1. Usage : CALL HC_HVPVET(ICN,T,HVP,IST)
2. Arguments

ICN : Component ID number (1-50) to calculate vapor pressure
(integer, input)

T : Temperature in Kelvin (real*8, input)

HVP : Heat of Vaporization in kJ/kg-mol (real*8, output)

IST : Status of calculation (integer, output)

= 0 : Normal termination

= 211 : Boiling point data not available

= 212 : Critical temperature data not available

= 213 : Critical pressure data not available

= 214 : Given T exceeds critical temperatue

3. Required Properties

Critical temperature in K, normal boiling temperature in K, and critical pressure in kPa.

4. Comments

For alcohols, specify ICLASS(ICN) as a value of 11 - 14 (See Description of common block in KDBROUTINE.PDF)