

NOTE: The following information is for Pure Compounds only. We are working on similar information for Binary Mixtures.

 trc.nist.gov/TDE/Equations/FEquations.html

Fitted Equations for Specific Properties

Listed below are the properties for which evaluated data is generated by *TDE*. Each property is linked to a list showing the set of possible equations that can be fit to the data. The equation that is used for a specific query is the one that provides the best fit of the data. This equation is then used to provide evaluated data.

NOTE: All of this information is displayed here in an individual file so that you can do text searches by using the **Find** function from the **Edit** menu of your browser.

Purpose: Provide definitions of equations and equation parameters used for output of evaluated data.

Select a property to see all associated equations. Properties represented with equations in *TDE* output are:

Vapor Pressure: *Liquid-Gas Phase Boundary Pressure*

- **DEFAULT: Wagner 25** ([sample parameter output](#))
 $\ln(p/p^o) - \ln(p_c/p^o) = T_c/T (A_1 + A_2 \times t^{1.5} + A_3 \times t^{2.5} + A_4 \times t^5)$; where $t = 1 - T/T_c$ and $p^o = 1$ kPa
- **Alternative 1: Antoine** ([sample parameter output](#))
 $\ln(p/p^o) = A + B/(T + C)$; where $p^o = 1$ kPa
- **Alternative 2: Yaws.VaporPressure** ([sample parameter output](#))
 $\lg(p/p^o) = a + b/T + c \times \lg(T) + d \times T + e/T^2$; where $p^o = 1$ kPa and $\lg = \log_{10}$
- **Alternative 3: DIPPR 115** ([sample parameter output](#))
 $\ln(p/p^o) = a + b/T + c \times \ln(T) + d \times T^2 + e/T^2$; where $p^o = 1$ kPa
- **Alternative 4: DIPPR 101** ([sample parameter output](#))
 $\ln(p/p^o) = a + b/T + c \times \ln(T) + d \times T^e$; where $p^o = 1$ kPa
- **Alternative 5: Wagner 36** ([sample parameter output](#))
 $\ln(p/p^o) - \ln(p_c/p^o) = T_c/T (A_1 + A_2 \times t^{1.5} + A_3 \times t^3 + A_4 \times t^6)$; where $t = 1 - T/T_c$ and $p^o = 1$ kPa

Wagner 25 (Vapor Pressure: *Output Details*)

$\ln(p/p^o) - \ln(p_c/p^o) = T_c/T (A_1 + A_2 \times t^{1.5} + A_3 \times t^{2.5} + A_4 \times t^5)$; where $t = 1 - T/T_c$ and $p^o = 1$ kPa

Evaluation Results:

```

Phase boundary pressure (Liquid, Gas)
Equation: Wagner25
Constant parameters: 562.05 =  $T_c$ 
Fitted parameters:
8.49654 =  $\ln(p_c/p^o)$ 
-7.06031 =  $A_1$ 
1.66439 =  $A_2$ 
-1.96525 =  $A_3$ 
-3.62497 =  $A_4$ 
Covariance matrix
9.68585e-008 -1.70506e-005 2.19028e-005 0 0
-8.03891e-007 0.000166807 -0.000221529 0 0
1.03266e-006 -0.000221529 0.000296324 0 0
0 0 0 0
0 0 0 0

```

The example is for fitted vapor pressures for **benzene**.

Antoine (Vapor Pressure: *Output Details*)

$\ln(p/p^o) = A + B/(T + C)$; where $p^o = 1$ kPa

Evaluation Results:

The example is for fitted vapor pressures for **benzene**.

```

Phase boundary pressure (Liquid, Gas)
Equation: Antoine
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 0
Fitted parameters:
14.1351 = A
-2933.9 = B
-45.1635 = C
Covariance matrix
13892.7 -6.96636e+013 -2.38978e+015
-64.6583 3.34354e+011 1.18591e+013
-2218.07 1.18591e+013 4.38702e+014

```

Yaws (Vapor Pressure: *Output Details*)

$\lg(p/p^o) = a + b/T + c \times \lg(T) + d \times T + e/T^2$; where $p^o = 1$ kPa and $\lg = \log_{10}$

Evaluation Results:

```
Phase boundary pressure (Liquid, Gas)
Equation: Yaws.VaporPressure
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 0
Fitted parameters:
39.7918      = a
-2965.83     = b
-12.073      = c
0.0033269    = d
1.58609e-006 = e
Covariance matrix
270771 -1.22281e+010 -2.18765e+008 241474 -100.426
-6.37617e+006 2.88304e+011 5.1501e+009 -5.67615e+006 2357.18
-114072 5.1501e+009 9.21687e+007 -101771 42.3397
125.914 -5.67615e+006 -101771 112.584 -0.0469245
-0.0523661 2357.18 42.3397 -0.0469245 1.95938e-005
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

The example is for fitted vapor pressures for **benzene**.

DIPPR 115 (Vapor Pressure: *Output Details*)

$\ln(p/p^0) = a + b/T + c \times \ln(T) + d \times T^2 + e/T^2$; where $p^0 = 1$ kPa

Evaluation Results:

The example is for fitted vapor pressures for **benzene**.

```
Phase boundary pressure (Liquid, Gas)
Equation: Antoine
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 0
Fitted parameters:
14.1351      = A
-2933.9      = B
-45.1635     = C
Covariance matrix
13892.7 -6.96636e+013 -2.38978e+015
-64.6583 3.34354e+011 1.18591e+013
-2218.07 1.18591e+013 4.38702e+014
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

DIPPR 101 (Vapor Pressure: *Output Details*)

$\ln(p/p^o) = a + b/T + c \times \ln(T) + d \times T^e$; where $p^o = 1$ kPa

Evaluation Results:

```
Phase boundary pressure (Liquid, Gas)
Equation: DIPPR 101
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 0
Fitted parameters:
82.3782      = a
-6645.83     = b
-10.2814     = c
6.30845e-005 = d
1.70291      = e
Covariance matrix
436690 -9270.69 -59.726 0.00614766 -12.8972
-1.16782e+007 248264 1596.76 -0.163932 343.841
-75236.2 1596.76 10.2906 -0.0010598 2.22347
7.74415 -0.163932 -0.0010598 1.09688e-007 -0.000230219
-16246.5 343.841 2.22347 -0.000230219 0.483213
*****
```

The example is for fitted vapor pressures for **benzene**.

Wagner36 (Vapor Pressure: *Output Details*)

$\ln(p/p^o) - \ln(p_c/p^o) = T_c/T (A_1 + A_2 \times t^{1.5} + A_3 \times t^3 + A_4 \times t^6)$; where $t = 1 - T/T_c$ and $p^o = 1$ kPa

Evaluation Results:

```

Phase boundary pressure (Liquid, Gas)
Equation: Wagner36
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 562.05 = Tc
Fitted parameters:
8.49596 = ln(pc/po)
-6.97117 = A1
1.29856 = A2
-2.56942 = A3
-3.49547 = A4
Covariance matrix
0.00562964 -1.49654e-005 3.21257e-005 -4.42706e-005 8.96025e-005
-0.1566 0.0006035 -0.00139302 0.00219819 -0.00494742
0.336168 -0.00139302 0.00327375 -0.0053559 0.0124564
-0.463254 0.00219819 -0.0053559 0.00944699 -0.0236573
0.937613 -0.00494742 0.0124564 -0.0236573 0.0643669

```

The example is for fitted vapor pressures for **benzene**.

Sublimation Pressure: *Crystal-Gas Phase Boundary Pressure*

- **DEFAULT: PV Expansion:** (sample parameter output)
 $\ln(p/p^o) = a_1 + a_2/T + a_3 \times \ln(T) + a_4 \times T + a_5 \times T^2 + a_6 \times T^6 + a_7/T^4$
- **Alternative 1: Antoine** (sample parameter output)
 $\ln(p/p^o) = A + B/(T + C)$; where $p^o = 1$ kPa
- **Alternative 2: Yaws.VaporPressure** (sample parameter output)
 $\lg(p/p^o) = a + b/T + c \times \lg(T) + d \times T + e/T^2$; where $p^o = 1$ kPa and $\lg = \log_{10}$
- **Alternative 3: DIPPR 115** (sample parameter output)
 $\ln(p/p^o) = a + b/T + c \times \ln(T) + d \times T^2 + e/T^2$; where $p^o = 1$ kPa
- **Alternative 4: DIPPR 101** (sample parameter output)
 $\ln(p/p^o) = a + b/T + c \times \ln(T) + d \times T^e$; where $p^o = 1$ kPa

PV Expansion: Sublimation Pressure

$$\ln(p/p^o) = a_1 + a_2/T + a_3 \times \ln(T) + a_4 \times T + a_5 \times T^2 + a_6 \times T^6 + a_7/T^4$$

NOTE: The *TDE* program truncates this equation based upon the extent and quality of the fitted data.

```

Phase boundary pressure (Crystal 1, Gas)
Equation: PVExpansion
Constant parameters: 0
Fitted parameters:
23.7969 = a1
-11422 = a2
0.177978 = a3
Covariance matrix
4461.53 -1.65957e+007 -39956.7
-263379 9.8627e+008 2.35585e+006
-634.125 2.35585e+006 5680.43

```

Condensed Phase boundary pressure

- **DEFAULT: PolynomialPressure:** ([sample parameter output](#))
 $\ln(p/p^0) = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$
- **Alternative 1:**
There are no alternative equations for this property at this time.

PolynomialExpansion: Phase boundary pressure for the crystal/liquid boundary

$\ln(p/p^0) = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

```

Phase boundary pressure (Crystal 1, Liquid)
Equation: PolynomialPressure
Constant parameters: 0
Fitted parameters:
-370367 = a0
-882.688 = a1
7.937 = a2
Covariance matrix
15001 -1.50506e+008 253005
-101.1 1.0147e+006 -1706.36
0.169953 -1706.36 2.87055

```

The example is for fitted phase-boundary pressures for **benzene**.

Density of the Liquid (on the Liquid/Gas phase boundary): d_{sat}

- **VDNS Expansion:** (sample parameter output)

$$d_{sat} = d_c + a_1 \times t^{0.35} + \sum_{i=1}^{nTerms-1} a_{i+1} \times t^i, \text{ where the summation is from } i = 1 \text{ to } nTerms - 1.$$

d_c = the critical density and $t = 1 - T/T_c$, where T_c is the critical temperature.

- **Alternative 1: Rackett** (sample parameter output)

$$d_{sat} = d_c \times B^{-(1-T/T_c)^N}; \text{ where } T_c \text{ and } d_c \text{ are the critical temperature and critical density, respectively.}$$

- **Alternative 2: PPDS 10** (sample parameter output)

$$d_{sat} = d_c + a_1 \times t^{0.35} + a_2 \times t^{2/3} + a_3 \times t + a_4 \times t^{4/3};$$

d_c = the critical density and $t = 1 - T/T_c$, where T_c is the critical temperature.

- **Alternative 3: PPDS 17** (sample parameter output)

$$d_{sat} = (a_1 + a_2 \times t)^{-1} \cdot t^{2/7} / a_0; \text{ where } t = 1 - T/T_c \text{ and } T_c \text{ is the critical temperature.}$$

VDNS Expansion: For d_{sat} of the Liquid or Gas phase

$$d_{sat} = d_c + a_1 \times t^{0.35} + \sum_{i=1}^{nTerms-1} a_{i+1} \times t^i; \text{ where the summation is from } i = 1 \text{ to } nTerms - 1.$$

d_c = the critical density and $t = 1 - T/T_c$, where T_c is the critical temperature.

Density (Liquid, Gas)	
Equation: VDNSExpansion	
Constant parameters: 748.402 314.629	= T_c and d_c
Fitted parameters:	
656.716	= a_1
336.778	= a_2
-214.225	= a_3
135.106	= a_4
Covariance matrix	
1551.14 -55864.1 106403 -78518.5	
-6095.58 224760 -440681 332675	
11610 -440681 894137 -692699	
-8567.49 332675 -692699 546915	

NOTE: The TDE program truncates this equation based upon the extent and quality of the fitted data.

Rackett Equation: For d_{sat} of the Liquid phase

$$d_{sat} = d_c \times B^{-(1-T/T_c)^N}; \text{ where } T_c \text{ and } d_c \text{ are the critical temperature and critical density, respectively.}$$

Density (Liquid, Gas)
Equation: Rackett
Validity range
Temperature: 353.344 to 748.402 K
Constant parameters: 748.402 314.629
Fitted parameters:
0.257033
0.280338
Covariance matrix
6.40678e-007 -1.03801e-008
-3.98383e-006 6.58494e-008

$= T_c \text{ and } d_c$

$= B$

$= N$

PPDS 10: For d_{sat} of the Liquid phase

$$d_{sat} = d_c + a_1 t^{0.35} + a_2 t^{2/3} + a_3 t + a_4 t^{4/3};$$

d_c = the critical density and $t = 1 - T/T_c$, where T_c is the critical temperature.

Evaluation Results:

Density (Liquid, Gas)
Equation: PPDS 10
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 562.05 305.99
Fitted parameters:
568.706
262.807
-376.687
409.076
Covariance matrix
21479 -387814 581645 -291053
-94839.9 1.74088e+006 -2.64647e+006 1.33861e+006
142241 -2.64647e+006 4.06726e+006 -2.07515e+006
-71177 1.33861e+006 -2.07515e+006 1.06604e+006

$= T_c \text{ and } d_c$

$= a_1$

$= a_2$

$= a_3$

$= a_4$

The example is for fitted densities at vapor saturation for **benzene**.

PPDS 17: For d_{sat} of the Liquid phase

$$d_{sat} = (a_1 + a_2 t)^{-1} \cdot t^{2/7} / a_0; \text{ where } t = 1 - T/T_c, \text{ and } T_c \text{ is the critical temperature.}$$

Evaluation Results:

The example is for fitted densities at vapor saturation for **benzene**.

Density (Liquid, Gas)
Equation: PPDS 17
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 562.05 = T_c
Fitted parameters:
0.0115508 = a_0
0.281004 = a_1
-0.00635447 = a_2
Covariance matrix
2.38023e-006 -0.000117965 4.75012e-005
-3.88088e-005 0.00192822 -0.000786833
1.56272e-005 -0.000786833 0.000347144

Density of the Gas (*on the Liquid/Gas phase boundary*)

- **VDNSExpansion:** (sample parameter output)

$d_{sat} = d_c + a_1 \times t^{0.35} + \sum_{i=1}^{nTerms-1} a_{i+1} \times t^i$, where the summation is from $i = 1$ to $nTerms - 1$.

d_c = the critical density and $t = 1 - T/T_c$, where T_c is the critical temperature.

- **Alternative 1:** There are no alternative equations for this property at this time.

Density (*Liquid Phase*)

- **Tait Equation:** (sample parameter output)

$d = d_{sat} / [1 - c \times \ln\{(b + p) / (b + p_{sat})\}]$; where

$b = \sum_{i=1}^{nTerms} B_{i+1} \times t^i$, $c = \sum_{i=1}^{nTerms} C_{i+1} \times t^i$, and $t = (T - T_{center})/100$, where T_{center} is a constant parameter. Summations are from $i = 0$ to $(nTerms - 1)$, where $nTerms$ is the number of B or C terms.

d_{sat} = the density of the saturated liquid and p_{sat} = the saturation vapor pressure.

- **Alternative 1:** There are no alternative equations for this property at this time.

Tait Equation: Density (*Liquid Phase*)

$d = d_{sat} / [1 - c \times \ln\{(b + p) / (b + p_{sat})\}]$; where

$b = \sum_{i=1}^{nTerms} B_{i+1} \times t^i$, $c = \sum_{i=1}^{nTerms} C_{i+1} \times t^i$, and $t = (T - T_{center})/100$, where T_{center} is a constant parameter.

Summations are from $i = 0$ to $(nTerms - 1)$, where $nTerms$ is the number of B or C terms.

d_{sat} = the density of the saturated liquid and p_{sat} = the saturation vapor pressure.

Density (Liquid)	
Equation: Tait	
Constant parameters: 3 293.15	= number of C terms and T_{center}
Fitted parameters:	
0.196293	= C_1
-0.199341	= C_2
0.0722272	= C_3
293863	= B_1
-571856	= B_2
377404	= B_3
-72288.5	= B_4
Covariance matrix	
7.74116e-005 -0.00183698 0.000569923 1863.15 -2488.89 439.537 140.94	
-0.000107973 0.00271094 -0.000868159 -2499.42 3277.99 -309.551 -307.611	
3.34986e-005 -0.000868159 0.000287474 779.363 -1068.22 139.025 91.9369	
109.511 -2499.42 779.363 3.14745e+009 -4.9574e+009 1.99778e+009 -1.56057e+008	
-146.291 3277.99 -1068.22 -4.9574e+009 9.093e+009 -5.18789e+009 8.54819e+008	
25.8349 -309.551 139.025 1.99778e+009 -5.18789e+009 4.76989e+009 -1.18738e+009	
8.28409 -307.611 91.9369 -1.56057e+008 8.54819e+008 -1.18738e+009 3.56315e+008	

There are 3 C terms in the example

NOTE: All terms after the C terms are B terms

Density (Gas Phase)

- **DEFAULT: Virial Equation (VirialV):**

(sample parameter output)

$d = 1000 \times Mw / V_m$; where Mw is the molar mass and V_m is the molar volume.

$$Z = 1000 \times p \times V_m / (R \times T) = 1 + B/V_m + C/V_m^2,$$

where $B = \sum b_{i+1}/T^i$ and $C = \sum c_{i+1}/T^i$

- **Alternative 1:**

There are no alternative equations for this property at this time.

VirialV: For density of the gas phase.

$d = 1000 \times Mw / V_m$; where Mw is the molar mass and V_m is the molar volume.

$Z = 1000 \times p \times V_m / (R \times T) = 1 + B/V_m + C/V_m^2$, where $B = \sum b_{i+1}/T^i$ and $C = \sum c_{i+1}/T^i$

Evaluation Results:

Density (Gas)
Equation: VirialV
Constant parameters: 2 4
Fitted parameters:

Number of virial coefficients (1 or 2)

Number of terms in the expansion(s)

0.00236047 = b_1
-2.78835 = b_2
1008.36 = b_3
-144483 = b_4
3.24632e-005 = c_1
-0.0421292 = c_2
18.311 = c_3
-2661.51 = c_4

Covariance matrix

6.63762e-006	-0.280193	98.0512	-11169	1.75528e-006	-0.0022286	0.938993	-131.296
-0.00710501	301.997	-106313	1.21653e+007	-0.00210273	2.65735	-1116.06	155758
2.48634	-106313	3.76202e+007	-4.32223e+009	0.798181	-1005.88	421679	-5.87938e+007
-283.219	1.21653e+007	-4.32223e+009	4.98215e+011	-95.4183	120084	-5.0303e+007	7.01223e+009
4.45097e-008	-0.00210273	0.798181	-95.4183	5.08378e-008	-6.18186e-005	0.0251504	-3.42222
-5.6512e-005	2.65735	-1005.88	120084	-6.18186e-005	0.0752646	-30.6569	4176.15
0.0238106	-1116.06	421679	-5.0303e+007	0.0251504	-30.6569	12501.4	-1.70484e+006
-3.32936	155758	-5.87938e+007	7.01223e+009	-3.42222	4176.15	-1.70484e+006	2.32743e+008

The example is for fitted gas densities of **pentane**.

Enthalpy of Vaporization (*Liquid/Gas*)

- **DEFAULT: HVP Expansion:** (sample parameter output)

$\ln(H_{vap}/H_{vap}^0) = a_1 + \sum_{i=2}^{nTerms-1} a_i \times T_r^{i-1} \times \ln(1-T_r)$, where the summation is from $i = 2$ to $nTerms - 1$

$T_r = T/T_c$, T_c is the critical temperature, and $H_{vap}^0 = 1$ kJ/mol

- **Alternative 1: Yaws.VaporizationH** (sample parameter output)

$H_{vap} = A \times \{1 - (T/T_c)\}^n$

- **Alternative 2: PPDS 12** (sample parameter output)

$H_{vap}/R = a_1 \times t^{1/3} + a_2 \times t^{2/3} + a_3 \times t + a_4 \times t^2 + a_5 \times t^6$

where $t = 1 - T/T_c$, T_c is the critical temperature, and R is the gas constant.

HVPExpansion: For H_{vap} for the liquid-gas phase boundary

$\ln(H_{vap}/H_{vap}^0) = a_1 + \sum_{i=2}^{nTerms-1} a_i \times T_r^{i-1} \times \ln(1-T_r)$, where the summation is from $i = 2$ to $nTerms - 1$

$T_r = T/T_c$, T_c is the critical temperature, and $H_{vap}^0 = 1$ kJ/mol

Evaluation Results:

```

Enthalpy of vaporization or sublimation (Liquid, Gas)
Equation: HVPExpansion
Constant parameters: 562.05 =  $T_c$ 
Fitted parameters:
4.21204 =  $a_1$ 
1.94122 =  $a_2$ 
-2.50004 =  $a_3$ 
1.07003 =  $a_4$ 
Covariance matrix
0.0133972 0.902484 -0.00270306 2.22338e-006
0.0541771 3.66298 -0.011009 9.10445e-006
-0.000162267 -0.011009 3.31969e-005 -2.75971e-008
1.33472e-007 9.10445e-006 -2.75971e-008 2.31307e-011

```

The example is for fitted enthalpies of vaporization for **benzene**.

Yaws.VaporizationH: For H_{vap} for the liquid-gas phase boundary

$$H_{vap} = A \times \{1 - (T / T_c)\}^n$$

Evaluation Results:

```

Enthalpy of vaporization or sublimation (Liquid, Gas)
Equation: Yaws.VaporizationH
Validity range
Temperature: 143.479 to 470.008 K
Constant parameters: 470.008 =  $T_c$ 
Fitted parameters:
39.1846 =  $A$ 
0.388985 =  $n$ 
Covariance matrix
0.235652 25.0968
0.00466812 0.655047

```

The example is for fitted enthalpies of vaporization for **pentane**.

PPDS12: For H_{vap} for the liquid-gas phase boundary

$$H_{vap}/R = a_1 \times t^{1/3} + a_2 \times t^{2/3} + a_3 \times t + a_4 \times t^2 + a_5 \times t^6$$

where $t = 1 - T/T_c$, T_c is the critical temperature, and R is the gas constant.

Evaluation Results:

Enthalpy of vaporization or sublimation (Liquid, Gas)	
Equation: PPDS 12	
Validity range	
Temperature: 278.469 to 562.05 K	
Constant parameters: 562.05	= T_c
Fitted parameters:	
0.00171484	= a_1
0.0258604	= a_2
-0.0243564	= a_3
0.00740881	= a_4
0.00680068	= a_5
Covariance matrix	
370.329 -10779.2 11744 -4944.24 5519.68	
-1529.57 45339.3 -50131.9 21786.9 -25792.7	
1666.47 -50131.9 56089.9 -24996.1 30993.5	
-701.586 21786.9 -24996.1 11745.5 -16081	
783.241 -25792.7 30993.5 -16081 26922.4	

The example is for fitted enthalpies of vaporization for **benzene**.

C_{sat} (Liquid Phase)

- **DEFAULT: CSExpansion:** (sample parameter output)
 $C_{sat} = (\sum a_{i+1} \times t^i) + b/t$, where the summation is from $i = 0$ to $nTerms - 1$.
- **Alternative 2: Yaws.PolynomialExpansion** (sample parameter output)
 $C_{sat} = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$
- **Alternative 3: DIPPR.PolynomialExpansion** (sample parameter output)
 $C_{sat} = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$
- **Alternative 3: PPDS 15** (sample parameter output)
 $C_{sat} / R = a_0/t + a_1 + a_2 \times t + a_3 \times t^2 + a_4 \times t^3 + a_5 \times t^4$

where $t = 1 - T/T_c$, T_c is the critical temperature, and R is the gas constant.

CSExpansion: For C_{sat} of the Liquid phase

$C_{sat} = (\sum a_{i+1} \times t^i) + b/t$, where the summation is from $i = 0$ to $nTerms - 1$.

Evaluation Results:


```

Heat capacity at saturation pressure (Liquid, Gas)
Equation: CSExpansion
Constant parameters: 562.05 =  $T_c$ 
Fitted parameters:
1.65368 =  $a_1$ 
80.0983 =  $a_2$ 
0.129891 =  $a_3$ 
0.000150676 =  $b$ 
Covariance matrix
0.0362564 -40.0116 0.241545 -0.000404136
-0.786752 1637 -9.65765 0.0149397
0.00474953 -9.65765 0.0572012 -8.90147e-005
-7.94656e-006 0.0149397 -8.90147e-005 1.40187e-007

```

The example is for fitted heat capacities at vapor saturation for **benzene**.

Yaws.PolynomialExpansion: For C_{sat} of the liquid phase

$C_{sat} = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

```

Heat capacity at saturation pressure (Liquid, Gas)
Equation: Yaws.PolynomialExpansion
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 0
Fitted parameters:
107.721 =  $a_0$ 
-0.0329581 =  $a_1$ 
0.000425549 =  $a_2$ 
Covariance matrix
107.153 -11.2033 0.0157639
-0.617624 0.0649609 -9.20818e-005
0.000869045 -9.20818e-005 1.31751e-007

```

$nTerms = 3$
in this example

The example is for fitted heat capacities at vapor saturation for **benzene**.

DIPPR.PolynomialExpansion: For C_{sat} of the liquid phase

$C_{sat} = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

```

Heat capacity at saturation pressure (Liquid, Gas)
Equation: DIPPR.PolynomialExpansion
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 0
Fitted parameters:
107.721      = a0
-0.0329581   = a1
0.000425549  = a2
Covariance matrix
107.153 -11.2033 0.0157639
-0.617624 0.0649609 -9.20818e-005
0.000869045 -9.20818e-005 1.31751e-007

```

nTerms = 3
in this example

The example is for fitted heat capacities at vapor saturation for **benzene**.

PPDS 15: For C_{sat} of the liquid phase

$$C_{sat} / R = a_0/t + a_1 + a_2 \times t + a_3 \times t^2 + a_4 \times t^3 + a_5 \times t^4$$

where $t = 1 - T/T_c$, T_c is the critical temperature, and R is the gas constant.

Evaluation Results:

```

Heat capacity at saturation pressure (Liquid, Gas)
Equation: PPDS 15
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 562.05 = Tc
Fitted parameters:
0.198892     = a0
24.1389      = a1
-20.2301     = a2
5.72481      = a3
4.43613e-007 = a4
-3.10751e-007 = a5
Covariance matrix
0.792672 -233.773 2197.09 -8846.9 16022.3 -10750.6
-23.599 8396.85 -87027.3 371333 -698672 481691
221.792 -87027.3 964167 -4.29172e+006 8.31167e+006 -5.85247e+006
-893.079 371333 -4.29172e+006 1.96453e+007 -3.88099e+007 2.77407e+007
1617.43 -698672 8.31167e+006 -3.88099e+007 7.77979e+007 -5.6245e+007
-1085.26 481691 -5.85247e+006 2.77407e+007 -5.6245e+007 4.10346e+007

```

The example is for fitted heat capacities at vapor saturation for **benzene**.

$C_p^o(\text{Ideal Gas})$

- **DEFAULT: Wilhoit Equation**

$$C_p^o / R = a_0 + (a_1 / T^2) \times \exp(-a_2 / T) + a_3 \times y^2 + \{a_4 - a_5 / (T - a_7)^2\} \times y^8$$

where $y = (T - a_7) / (T + a_6)$ and R is the gas constant.

See *Thermodynamics of Organic Compounds in the Gas State (Volumes I and II)* by M. Frenkel, G. J. Kabo, K. N. Marsh, G. N. Roganov, and R. C. Wilhoit. Published by the Thermodynamics Research Center (TRC), College Station: TX. **1994**.

- **Alternative 1: Yaws.PolynomialExpansion** ([sample parameter output](#))

$$C_p^o = \sum a_i \times T^i, \text{ where the summation is from } i = 0 \text{ to } n\text{Terms} - 1$$

- **Alternative 2: AlyLee (which is also DIPPR 107)** ([sample parameter output](#))

$$C_p^o = a + b \times \{(c/T) / \sinh(c/T)\}^2 + d \times \{(e/T) / \cosh(e/T)\}^2$$

- **Alternative 3: PPDS2** ([sample parameter output](#))

$$C_p^o / R = C_{\text{low}} + (C_{\text{low}} - C_{\infty}) \times y^2 \times \{1 + (y - 1) \sum (a_i \times y_i)\}; \text{ where the summation is from } i = 0 \text{ to } 4.$$

C_{low} and C_{∞} are equation constants, and $y = T / (T + T_S)$, where T_S is a constant.

- **Alternative 4: Helmholtz** ([sample parameter output](#))

$$C_p^o / R = 1 + t - \{ \sum a_i \times n_i \times (n_i - 1) \times t^{n_i} \}_{(n_i \neq 0 \text{ or } 1)} + \sum b_i \times (c_i \times t)^2 \times \exp(c_i \times t) / \{ \exp(c_i \times t) - 1 \}^2;$$

where $t = T_c / T$, T_c = the critical temperature, and the summations are from $i = 1$ to $n\text{Terms}$.

$C_p^o(\text{Ideal Gas})$

$$C_p^o = \sum a_i \times T^i, \text{ where the summation is from } i = 0 \text{ to } n\text{Terms} - 1$$

```

Heat capacity at constant pressure (Ideal gas)
Equation: Yaws.PolynomialExpansion
Validity range
Temperature: 200 to 1500 K
Constant parameters: 0
Fitted parameters:
40.7159      = a0
0.215698    = a1
0.000294863 = a2
-3.94015e-007 = a3
1.25482e-010 = a4
Covariance matrix
21.4021 -1.33339 0.00306966 -2.72982e-006 8.21216e-010
-0.158965 0.0101917 -2.39768e-005 2.16559e-008 -6.58911e-012
0.000365961 -2.39768e-005 5.76874e-008 -5.30398e-011 1.6361e-014
-3.25446e-007 2.16559e-008 -5.30398e-011 4.95305e-014 -1.54741e-017
9.79045e-011 -6.58911e-012 1.6361e-014 -1.54741e-017 4.88721e-021

```

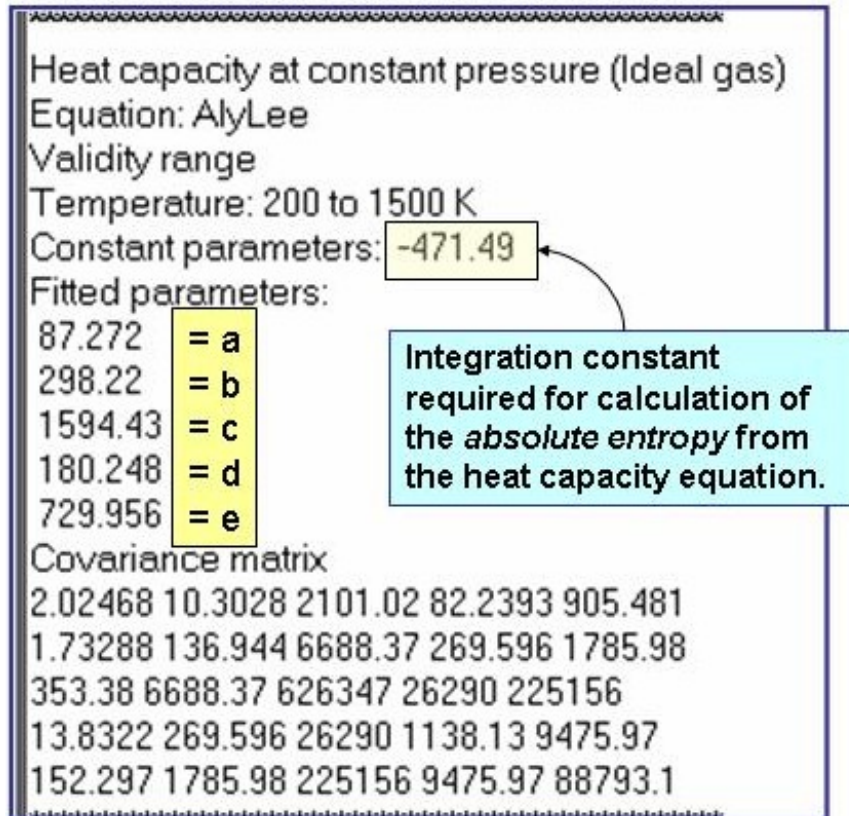
The example is for fitted heat capacities in the ideal-gas state at $p = 100$ kPa for **pentane**.

Aly & Lee Equation (same as DIPPR 107):

$C_p^\circ(\text{Ideal Gas})$

$$C_p^\circ = a + b \times \{(c/T)/\sinh(c/T)\}^2 + d \times \{(e/T)/\cosh(e/T)\}^2$$

Reference: Aly, F. A.; Lee, L. L. *Fluid Phase Equil.* **1981**, 6, 169-179.

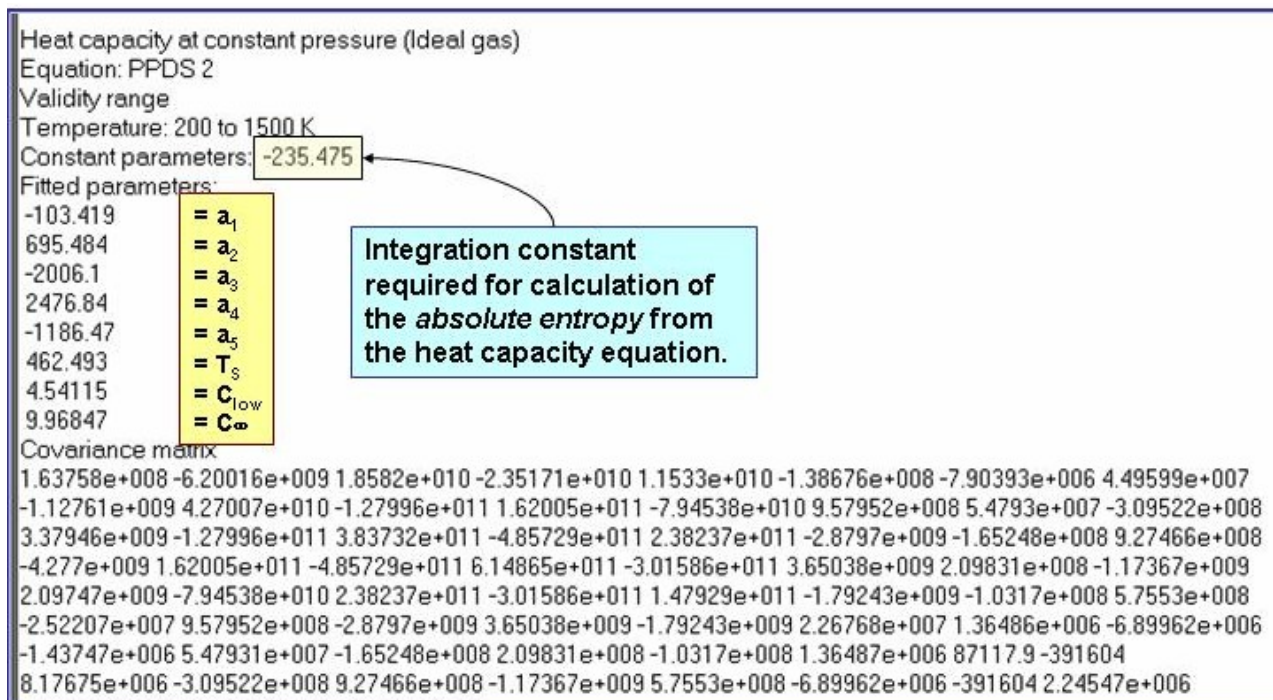


The example is for fitted heat capacities in the ideal-gas state at $p = 100$ kPa for **pentane**.

PPDS 2: $C_p^\circ(\text{Ideal Gas})$

$C_p^\circ/R = C_{\text{low}} + (C_{\text{low}} - C_\infty) \times y^2 \times \{1 + (y - 1) \sum_{i=0}^4 a_i \times y_i\}$; where the summation is from $i = 0$ to 4.
 C_{low} and C_∞ are equation constants, and $y = T / (T + T_s)$, where T_s is a constant.

Evaluation Results:



The example is for fitted heat capacities in the ideal-gas state at $p = 100$ kPa for **pentane**.

Helmholtz: $C_p^\circ(\text{Ideal Gas})$

$C_p^\circ/R = 1 + t - \{a_i \times n_i \times (n_i - 1) \times t^{n_i}\}_{(n_i: 0 \text{ or } 1)} + \{b_i \times (c_i \times t)^2 \times \exp(c_i \times t) / \{\exp(c_i \times t) - 1\}^2\}$
 where $t = T_c/T$, T_c = the critical temperature, and the summations are from $i = 1$ to $n\text{Terms}$.

Heat capacity at constant pressure (Ideal gas)

Equation: HelmholtzIG

Validity range

Temperature: 50 to 1500 K

Constant parameters: 1 2 -27.6743

Fitted parameters:

2.88938	= t
-4.53889	= a ₁
-1.10044	= n
9.92058	= b ₁
1.8361	= c ₁
-27.4747	= b ₂
9.24628	= c ₂

Covariance matrix

0.0127808	0.0196233	-0.00438098	-0.0353189	-0.00326349	-0.282996	-0.0144027
0.0349232	0.0601826	-0.0111318	-0.0688524	-0.00932237	-0.694057	-0.0221507
-0.00779674	-0.0111318	0.00333636	0.0350044	0.00236087	0.229259	0.0152768
-0.0628563	-0.0688524	0.0350044	0.486991	0.0241281	2.69243	0.192211
-0.00580796	-0.00932237	0.00236087	0.0241281	0.00217781	0.172223	0.00593521
-0.503642	-0.694057	0.229259	2.69243	0.172223	19.0515	0.696171
-0.0256323	-0.0221507	0.0152768	0.192211	0.00593521	0.696171	0.175652

Integration constant required for calculation of the **absolute entropy** from the heat capacity equation.

Number of **a** terms (1 here) and **b** and **c** terms (2 each here) in the summations.

The example is for fitted heat capacities in the ideal-gas state at $p = 100$ kPa for **2-methylpyrrole**.

Speed of Sound (*Liquid Phase*)

- **DEFAULT: RSSL Expansion:** (sample parameter output)

$$u = A + B \times T + C \times (d - d_{sat}) + D \times d^2,$$

where d is the density of the liquid and d_{sat} is the density of the saturated liquid.

- **Alternative 1:**

There are no alternative representations for this property at this time.

Speed of Sound (*Liquid Phase*)

$$u = A + B \times T + C \times (d - d_{sat}) + D \times d^2,$$

where d is the density of the liquid and d_{sat} is the density of the saturated liquid.

Speed of sound (Liquid)	
Equation: RSSLExpansion	
Constant parameters: 0	
Fitted parameters:	
17903	= A
-26.3217	= B
26.5673	= C
-0.0114629	= D
Covariance matrix	
1.45065e+007	-137189 130180 -73.293
-20550.5	194.379 -184.408 0.103818
19500.5	-184.408 175.021 -0.0985291
-10.9791	0.103818 -0.0985291 5.54758e-005

The example is for fitted speeds of sound for **benzene**.

Speed of Sound (*Gas Phase*)

- **DEFAULT: RSSG Expansion:** (sample parameter output)

$$u = A + B \times T + C \times p + D \times p/T;$$

where T is the temperature and p is pressure.

- **Alternative 1:**

There are no alternative representations for this property at this time.

Speed of Sound (*Gas Phase*)

$$u = A + B \times T + C \times p + D \times p/T;$$

where T is the temperature and p is pressure.

```

Speed of sound (Gas)
Equation: RSSGExpansion
Constant parameters: 0
Fitted parameters:
99.8061      = A
0.309375    = B
0.0389746   = C
-34.1738    = D
Covariance matrix
40.5054 -0.00555531 0.0430804 -12.9499
-0.137664 1.90059e-005 -0.000137036 0.0407235
1.06756 -0.000137036 0.00318247 -1.01291
-320.907 0.0407235 -1.01291 323.779

```

The example is for fitted speeds of sound for **pentane** in the gas phase.

Refractive Index n_D (Liquid)

- **DEFAULT: RIXExpansion:** ([sample parameter output](#))

$$n_D = A + B \times t + \sum C_i \times w^i ; \text{the summation is from } i = 1 \text{ to } nTerms$$

where $t = T - 298.15$ K and $w = WL - 589.26$ (WL = wavelength in nm)

- **Alternative 1:**

There are no alternative equations for this property at this time.

RIXExpansion: *Refractive Index n_D (Liquid)*

$$n_D = A + B \times t + \sum C_i \times w^i ; \text{the summation is from } i = 1 \text{ to } nTerms$$

where $t = T - 298.15$ K and $w = WL - 589.26$ (WL = wavelength in nm)

Evaluation Results:

```

Refractive index (Liquid)
Equation: RIXExpansion
Constant parameters: 0
Fitted parameters:
1.35476      = A
-0.000570369 = B
-3.39562e-005 = C1
5.83357e-008  = C2
Covariance matrix
3.69579e-008 2.72393e-009 9.2519e-011 -4.83171e-014
4.42263e-009 1.257e-009 7.9979e-012 1.2972e-013
1.50216e-010 7.9979e-012 1.39977e-011 -3.31759e-014
-7.84487e-014 1.2972e-013 -3.31759e-014 1.40697e-016

```

The example is for fitted surface tensions for **pentane**.

Surface Tension s (*Liquid/Gas*)

- **DEFAULT: PPDS 14:** ([sample parameter output](#))
 $s = a_0 \times t^{a_1} \times (1 + a_2 \times t)$, where $t = 1 - T/T_c$ and T_c is the critical temperature.
- **Alternative 1: Yaws.SurfaceTension** ([sample parameter output](#))
 $s = \exp(A) \times \{1 - (T/T_c)\}^n$
- **Alternative 2: HVPExpansion** ([sample parameter output](#))
 $\ln(s/s^0) = a_1 + \sum a_i \times T_r^{i-1} \times \ln(1-T_r)$, where the summation is from $i = 2$ to $nTerms - 1$
 $T_r = T/T_c$, T_c is the critical temperature, and $s^0 = 1 \text{ N/m}$

PPDS14: For surface tension s for the liquid/gas interface

$s = a_0 \times t^{a_1} \times (1 + a_2 \times t)$, where $t = 1 - T/T_c$ and T_c is the critical temperature.

Evaluation Results:

The example is for fitted surface tensions for **benzene**.

```

Surface tension (Liquid, Gas)
Equation: PPDS 14
Constant parameters: 562.05 =  $T_c$ 
Fitted parameters:
0.0786269 =  $a_0$ 
1.28646 =  $a_1$ 
-0.112304 =  $a_2$ 
Covariance matrix
1.41709e-005 0.463352 -1.29775
8.4683e-005 2.82555 -7.65131
-0.000237179 -7.65131 21.9504

```

Yaws.SurfaceTension: *For surface tension s for the liquid/gas interface*

- **Alternative 1: Yaws.SurfaceTension** (sample parameter output)

$$s = \exp(A) \times \{1 - (T / T_c)\}^n$$

Evaluation Results:

The example is for fitted surface tensions for **benzene**.

```

Surface tension (Liquid, Gas)
Equation: Yaws.SurfaceTension
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 562.05 =  $T_c$ 
Fitted parameters:
0.0725629 =  $A$ 
1.25018 =  $n$ 
Covariance matrix
3.84945 0.00265027
52.834 0.0397931

```

HVPExpansion: *For surface tension s for the liquid/gas interface*

$\ln(s/s^0) = a_1 + \sum_{i=2}^{nTerms-1} a_i \times T_r^{i-1} \times \ln(1-T_r)$, where the summation is from $i = 2$ to $nTerms - 1$
 $T_r = T/T_c$, T_c is the critical temperature, and $s^0 = 1 \text{ N/m}$

The example is for fitted surface tensions for **benzene**.

```

Surface tension (Liquid, Gas)
Equation: HVPExpansion
Validity range
Temperature: 278.469 to 562.05 K
Constant parameters: 562.05 =  $T_c$ 
Fitted parameters:
-2.52566 =  $a_1$ 
1.90209 =  $a_2$ 
-1.71734 =  $a_3$ 
1.70584 =  $a_4$ 
-0.60242 =  $a_5$ 
Covariance matrix
243.805 7553.28 -19580 20405.2 -8104.02
1434.43 44640.6 -116076 121305 -48264.6
-3718.41 -116076 302468 -316717 126181
3875.11 121305 -316717 332250 -132538
-1539.02 -48264.6 126181 -132538 52920.3

```

Viscosity (*Saturated Liquid*)

- **DEFAULT: PPDS 9:** ([sample parameter output](#))
 $\ln(h/h^0) = a_1 \times X^{1/3} + a_2 \times X^{4/3} + \ln(a_5)$, where $X = (a_3 - T) / (T - a_4)$ and $h^0 = 1 \text{ Pa}\cdot\text{s}$
- **Alternative 1: Yaws.Viscosity** ([sample parameter output](#))
 $\lg(h/h^0) = A + B/T + C \times T + D \times T^2$
- **Alternative 2: DIPPR 101** ([sample parameter output](#))
 $\ln(h/h^0) = a + b/T + c \times \ln(T) + d \times T^e$; where $h^0 = 1 \text{ Pa}\cdot\text{s}$

PPDS9: Viscosity h of the saturated liquid

$\ln(h/h^0) = a_1 \times X^{1/3} + a_2 \times X^{4/3} + \ln(a_5)$, where $X = (a_3 - T) / (T - a_4)$ and $h^0 = 1 \text{ Pa}\cdot\text{s}$.

Evaluation Results:

```

Viscosity (Liquid, Gas)
Equation: PPDS 9

Fitted parameters:
6.95415e-006 = a1
3.10203      = a2
0.00700796  = a3
718.36       = a4
155.023      = a5

Covariance matrix
2.96001e-010 0.00111834 0.00247464 -0.230745 -1.2202
2.6623e-005 120.725 247.966 -20063.9 -122748
5.89107e-005 247.966 524.673 -45018.6 -259310
-0.00549308 -20063.9 -45018.6 4.31402e+006 2.2182e+007
-0.0290478 -122748 -259310 2.2182e+007 1.2817e+008

```

The example is for fitted viscosities for the saturated liquid phase of **benzene**.

Yaws.Viscosity: *Viscosity h of the saturated liquid*

$$\lg(h/h^\circ) = A + B/T + C \times T + D \times T^2$$

Evaluation Results:

```

Viscosity (Liquid, Gas)
Equation: Yaws.Viscosity
Validity range
Temperature: 280.819 to 560 K
Constant parameters: 0
Fitted parameters:
-6.61826      = A
716.336       = B
0.00480826    = C
-4.87187e-006 = D

Covariance matrix
171.71 -26590.6 -0.560776 0.000480607
-21364.7 3.31947e+006 69.5422 -0.0594083
-0.450566 69.5422 0.00147651 -1.26973e-006
0.000386153 -0.0594083 -1.26973e-006 1.09568e-009

```

The example is for fitted viscosities for the saturated liquid phase of **benzene**.

DIPPR101: *Viscosity h of the saturated liquid*

$\ln(h/h^0) = a + b/T + c \times \ln(T) + d \times T^e$; where $h^0 = 1 \text{ Pa} \times s$

Evaluation Results:

```
Viscosity (Liquid, Gas)
Equation: DIPPR 101
Validity range
Temperature: 280.819 to 560 K
Constant parameters: 0
Fitted parameters:
-114.835 = A
4411.61 = B
57.0356 = C
-74.3069 = D
0.200078 = E
Covariance matrix
2.07392e+009 1.13877e+010 1.08354e+009 -4.61094e+009 -3.69908e+006
7.13848e+009 3.93332e+010 3.73279e+009 -1.58788e+010 -1.27366e+007
6.79223e+008 3.73279e+009 3.54943e+008 -1.5103e+009 -1.21157e+006
-2.8904e+009 -1.58788e+010 -1.5103e+009 6.42667e+009 5.15561e+006
-2.31879e+006 -1.27366e+007 -1.21157e+006 5.15561e+006 4135.97
```

The example is for fitted viscosities for the saturated liquid phase of **benzene**.

Viscosity (*Gas at low pressures; $p < 6 \text{ bar}$*)

- **DEFAULT: TransportPolynomial:** (sample parameter output)
 $h = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$
- **Alternative 1: Yaws.PolynomialExpansion** (sample parameter output)
 $h = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$
- **Alternative 2: DIPPR 102** (sample parameter output)
 $h = A \times T^B / (1 + C/T + D/T^2)$
- **Alternative 3: PPDS 5** (sample parameter output)
 $h = a_0 \times T_r / \{1 + a_1 \times (T_r - 1) \times T_r^{a_2}\}^{1/6}$; where $T_r = T/T_c$ and T_c is the critical temperature.

TransportPolynomial: *For viscosity h of the gas at low pressures ($p < 600 \text{ kPa}$)*

$h = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

```

Viscosity (Gas)
Equation: TransportPolynomial
Constant parameters:
Fitted parameters:
-1.99885e-007 = a0
2.45835e-008 = a1
-2.51091e-012 = a2
Covariance matrix
2.8015e-012 -1.15039e-013 1.39852e-016
-1.38755e-014 5.7239e-016 -6.98908e-019
1.68685e-017 -6.98908e-019 8.57207e-022

```

The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

Yaws.PolynomialExpansion: *For viscosity h of the gas at low pressures ($p < 600$ kPa)*

$h = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

```

Viscosity (Gas)
Equation: Yaws.PolynomialExpansion
Validity range
Temperature: 324.137 to 579.011 K
Pressure: 0 to 0 kPa
Constant parameters: 0
Fitted parameters:
-1.99885e-007 = a0
2.45835e-008 = a1
-2.51091e-012 = a2
Covariance matrix
2.53439e-012 -4.70583e-014 5.5828e-017
-1.22265e-014 2.28246e-016 -2.72205e-019
1.4505e-017 -2.72205e-019 3.26386e-022

```

DIPPR 102: *For viscosity h of the gas at low pressures ($p < 600$ kPa)*

$h = A \times T^B / (1 + C/T + D/T^2)$

Evaluation Results:


```

Viscosity (Gas)
Equation: DIPPR 102
Validity range
Temperature: 324.137 to 579.011 K
Pressure: 0 to 0 kPa
Constant parameters: 0
Fitted parameters:
9.15041e-008 = A
0.808921 = B
123.924 = C
-7666.64 = D
Covariance matrix
1.19137e-011 -6.49846e-005 0.0702446 -5.52758
-1.6884e-005 92.0988 -99530.7 7.82974e+006
0.0182506 -99530.7 1.07728e+008 -8.49207e+009
-1.43615 7.82974e+006 -8.49207e+009 6.71289e+011

```

The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

PPDS 5: *For viscosity η of the gas at low pressures ($p < 600$ kPa)*

$\eta = a_0 \times T_r / \{1 + a_1 \times (T_r - 1) \times T_r^{a_2}\}^{1/6}$; where $T_r = T/T_c$ and T_c is the critical temperature.

Evaluation Results:

```

Viscosity (Gas)
Equation: PPDS 5
Validity range
Temperature: 324.137 to 579.011 K
Pressure: 0 to 0 kPa
Constant parameters: 470.008 =  $T_c$ 
Fitted parameters:
1.08003e-005 =  $a_0$ 
0.19583 =  $a_1$ 
0.811897 =  $a_2$ 
Covariance matrix
3.33044e-015 -7.37579e-014 4.30419e-012
-2.63327e-014 2.95915e-011 4.39077e-010
1.53666e-012 4.39077e-010 1.31689e-008

```

The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

Thermal Conductivity I: (Liquid)

- **DEFAULT: TransportPolynomial:** (sample parameter output)

$I = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

- **Alternative 1: Yaws.ThermalConductivity** (sample parameter output)

$\lg(I/I^\circ) = A + B \times (1 - T/C)^{2/7}$

- **Alternative 2: Yaws.PolynomialExpansion** (sample parameter output)

$I = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

- **Alternative 3: DIPPR.PolynomialExpansion** (sample parameter output)

$I = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

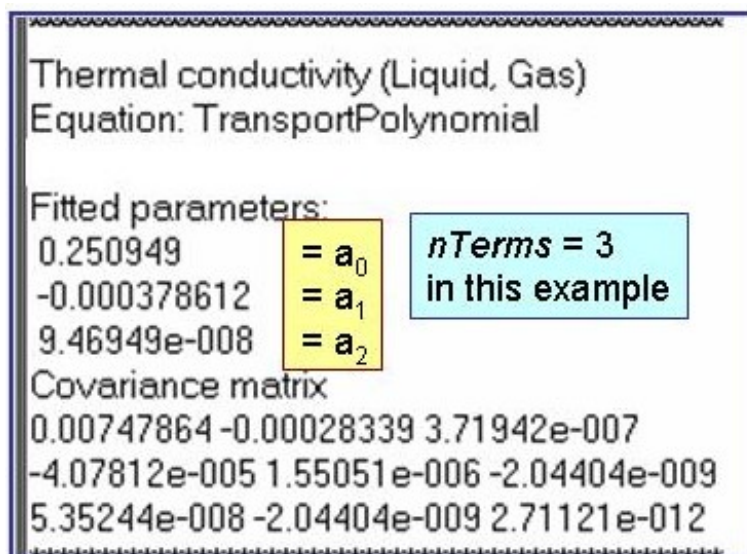
- **Alternative 4: PPDS 8** (sample parameter output)

$I = a_1 + \sum (a_{i+1} \times t^{i/3})$, where the summation is from $i = 1$ to $nTerms - 1$ and $t = 1 - T/T_c$

TransportPolynomial: For thermal conductivity I of the saturated liquid

$I = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:



The example is for fitted thermal conductivities for the saturated liquid phase of **benzene**.

Yaws.ThermalConductivity: For thermal conductivity I of the saturated liquid

$\lg(I/I^\circ) = A + B \times (1 - T/C)^{2/7}$

Evaluation Results:

The example is for fitted thermal conductivities for the saturated liquid phase of **benzene**.

```

Thermal conductivity (Liquid, Gas)
Equation: Yaws.ThermalConductivity
Validity range
Temperature: 270 to 550.809 K
Constant parameters:
Fitted parameters:
-1.56779 = A
0.904537 = B
562.05 = C
Covariance matrix
12.6394 -0.303357 -4.23896e-005
-14.4343 0.347516 4.76397e-005
-0.00201697 4.76397e-005 7.54707e-009

```

Yaws.PolynomialExpansion: *For thermal conductivity I of the saturated liquid*

$I = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

The example is for fitted thermal conductivities for the saturated liquid phase of **benzene**.

```

Thermal conductivity (Liquid, Gas)
Equation: Yaws.PolynomialExpansion
Validity range
Temperature: 270 to 562.05 K
Constant parameters: 0
Fitted parameters:
0.250949 = a0
-0.000378612 = a1
9.46949e-008 = a2
Covariance matrix
0.00405839 -0.000147328 1.93209e-007
-2.20209e-005 8.04189e-007 -1.0616e-009
2.88786e-008 -1.0616e-009 1.41264e-012

```

$nTerms = 3$
in this example

DIPPR.PolynomialExpansion: *For thermal conductivity I of the saturated liquid*

$I = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

The example is for fitted thermal conductivities for the saturated liquid phase of **benzene**.

```

Thermal conductivity (Liquid, Gas)
Equation: DIPPR.PolynomialExpansion
Validity range
Temperature: 270 to 562.05 K
Constant parameters: 0
Fitted parameters:
0.250949 = a0
-0.000378612 = a1
9.46949e-008 = a2
Covariance matrix
0.00405839 -0.000147328 1.93209e-007
-2.20209e-005 8.04189e-007 -1.0616e-009
2.88786e-008 -1.0616e-009 1.41264e-012
  
```

nTerms = 3
in this example

PPDS8: For thermal conductivity l of the saturated liquid

$l = a_1 + \sum (a_{i+1} \times t^{i/3})$, where the summation is from $i = 1$ to **nTerms - 1** and $t = 1 - T/T_c$

Evaluation Results:

The example is for fitted thermal conductivities for the liquid phase of **benzene**.

```

Thermal conductivity (Liquid, Gas)
Equation: PPDS 8
Validity range
Temperature: 270 to 562.05 K
Constant parameters: 562.05 = Tc
Fitted parameters:
0.0641126 = a1
0.61057 = a2
-1.72442 = a3
3.94394 = a4
Covariance matrix
0.0101735 -6.8731 12.768 -10.4908
-0.976437 704.905 -1358.8 1103.87
1.8139 -1358.8 2673.5 -2161.56
-1.49039 1103.87 -2161.56 1751.7
  
```

Thermal Conductivity (Gas at low pressures; $p < 6$ bar)

- **DEFAULT: TransportPolynomial:** (sample parameter output)

$l = \sum a_i \times T^i$, where the summation is from $i = 0$ to **nTerms - 1**

- **Alternative 1: Yaws.PolynomialExpansion** (sample parameter output)

$l = \sum a_i \times T^i$, where the summation is from $i = 0$ to **nTerms - 1**

- **Alternative 2: PPDS 3** (sample parameter output)

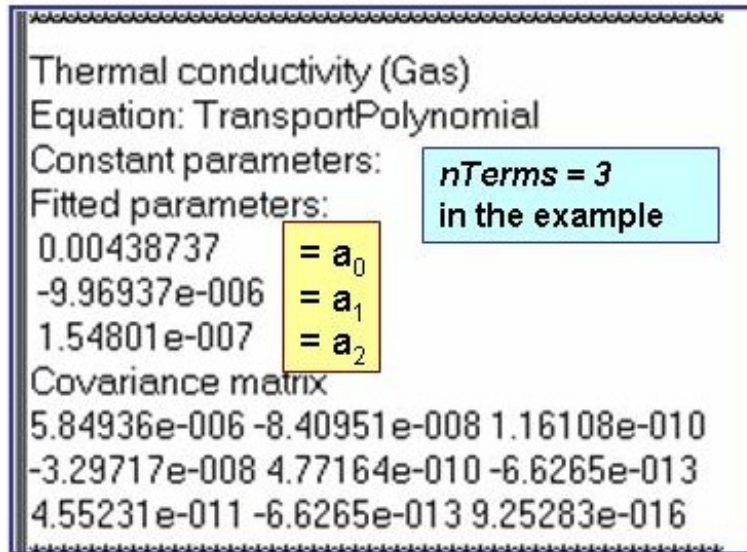
$\lambda = T_r^{0.5} (\sum a_i / T_r^i)^{-1}$, where the summation is from $i = 1$ to 3 ,

and $T_r = T/T_c$, where T_c is the critical temperature.

TransportPolynomial: *For thermal conductivity λ of the gas at low pressure ($p < 600$ kPa)*

$\lambda = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:



The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

Yaws.PolynomialExpansion: *For thermal conductivity λ of the gas at low pressure ($p < 600$ kPa)*

$\lambda = \sum a_i \times T^i$, where the summation is from $i = 0$ to $nTerms - 1$

Evaluation Results:

The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

Thermal conductivity (Gas)
Equation: Yaws.PolynomialExpansion
Validity range
Temperature: 277.594 to 444.223 K
Pressure: 0 to 0 kPa
Constant parameters: 0
Fitted parameters:
0.00438737 = a_0
-9.96937e-006 = a_1
1.54801e-007 = a_2
Covariance matrix
2.57065e-006 -4.51384e-008 6.24569e-011
-1.44412e-008 2.5461e-010 -3.53621e-013
1.99819e-011 -3.53621e-013 4.92911e-016

PPDS 3: For thermal conductivity I of the gas at low pressure ($p < 600$ kPa)

$I = T_r^{0.5} (\sum a_i / T_r^i)^{-1}$, where the summation is from $i = 1$ to 3 ,
and $T_r = T/T_c$, where T_c is the critical temperature.

Evaluation Results:

The example is for fitted thermal conductivities for the saturated liquid phase of **pentane**.

Thermal conductivity (Gas)
Equation: PPDS 3
Validity range
Temperature: 277.594 to 444.223 K
Pressure: 0 to 0 kPa
Constant parameters: 470.008 = T_c
Fitted parameters:
11.6366 = a_1
25.1191 = a_2
-7.21674 = a_3
Covariance matrix
0 0 -0.981347
0 0 -0.981347
1 0.981347 0.00816144