根据CAS号, 从数据库中找到对应物质的物性数据

以苯为例子, CAS = 71-43-2

```
CAS = '71-43-2';
C6H6 = Component(CAS);
```

- Ename, 英文名字, -

```
Ename = C6H6.Ename
```

```
Ename =
'Benzene'
```

- Pc, 临界压力, Pa

```
Pc = C6H6.Pc
```

```
Pc = 4895000
```

- Tc, 临界温度, K

```
Tc = C6H6.Tc
```

```
Tc = 562.0500
```

- Vc, 临界体积, $\frac{m^3}{\mathrm{kmol}}$

```
Vc = C6H6.Vc
```

```
Vc = 0.2560
```

- Zc, 临界压缩因子, -

```
Zc = C6H6.Zc
```

```
Zc = 0.2680
```

- Tb, 常压沸点温度, K

```
Tb = C6H6.Tb
```

```
Tb = 353.2400
```

- Ttriple, 三相点温度, K

```
Ttriple = C6H6.Ttriple
```

```
Ttriple = 278.6800
```

- Ptriple, 三相点压力, Pa

```
Ptriple = C6H6.Ptriple
```

```
Ptriple = 4.7642e+03
```

- Mw, 摩尔质量, $\frac{\mathrm{kg}}{\mathrm{kmol}}$

```
Mw = C6H6.Mw
```

```
Mw = 78.1140
```

- ω，偏心因子, -

```
Omega = C6H6.Omega
```

```
Omega = 0.2090
```

- H^m_{form}，标准摩尔生成焓, $\frac{J}{\mathrm{kmol}}$

```
Hfrom = C6H6.Hform
```

```
Hfrom = 82880000
```

- G^m_{from}，标准摩尔生成自由能, $\frac{J}{\mathrm{kmol}}$

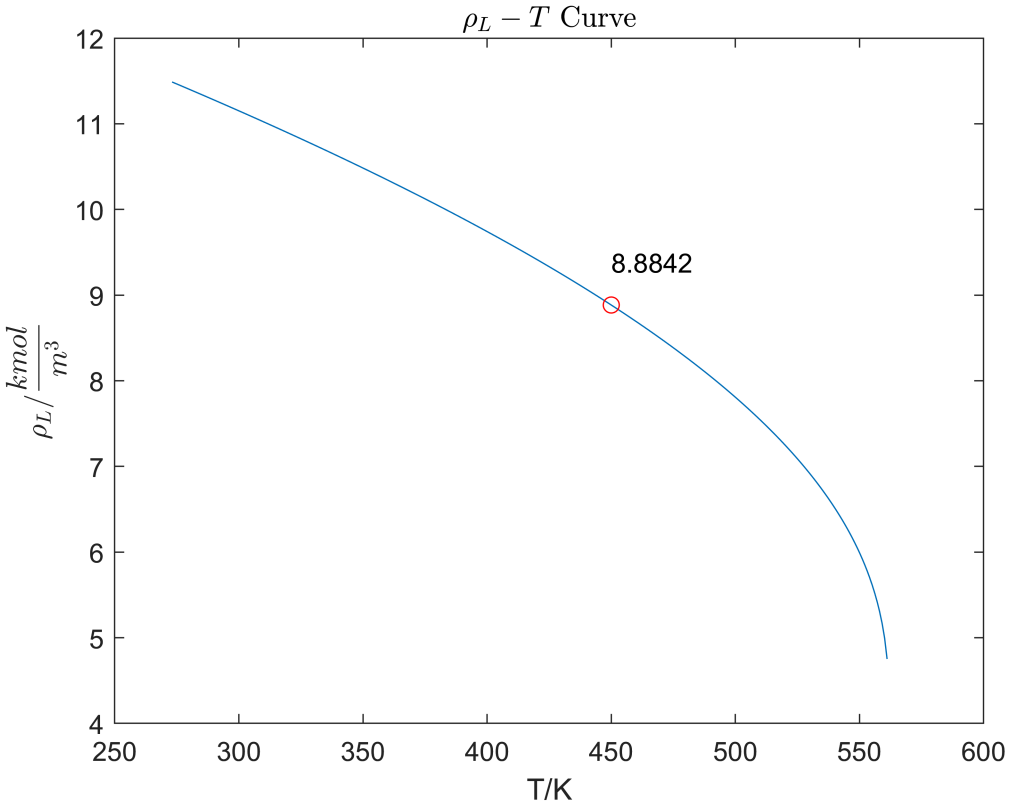
```
Gform = C6H6.Gform
```

```
Gform = 129600000
```

- LiquidDensity, 液体的密度, kmol/m^3

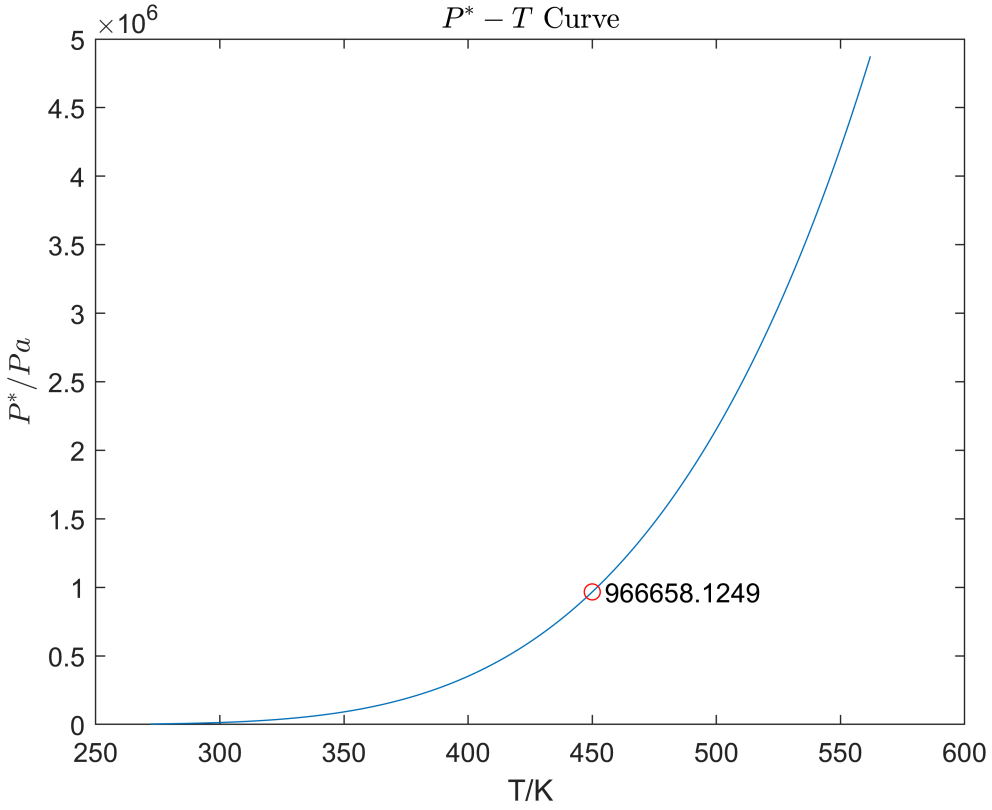
- $\rho_L = \frac{A}{B^{\left(1+\left(1-\frac{T}{C}\right)^{D}\right)}}$

```
plot([ C6H6.LiquidDensity(end-1):C6H6.LiquidDensity(end) ], C6H6.LiquidDensity_func( [C6H6.Liqu
hold on
plot(450,  C6H6.LiquidDensity_func(450), 'or')
text(450,  C6H6.LiquidDensity_func(450)+0.5, num2str(C6H6.LiquidDensity_func(450)) )
hold off
title('$${\rho_L-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${ \rho_L/ \frac{kmol}{m^3} }$$', 'Interpreter', 'latex')
```



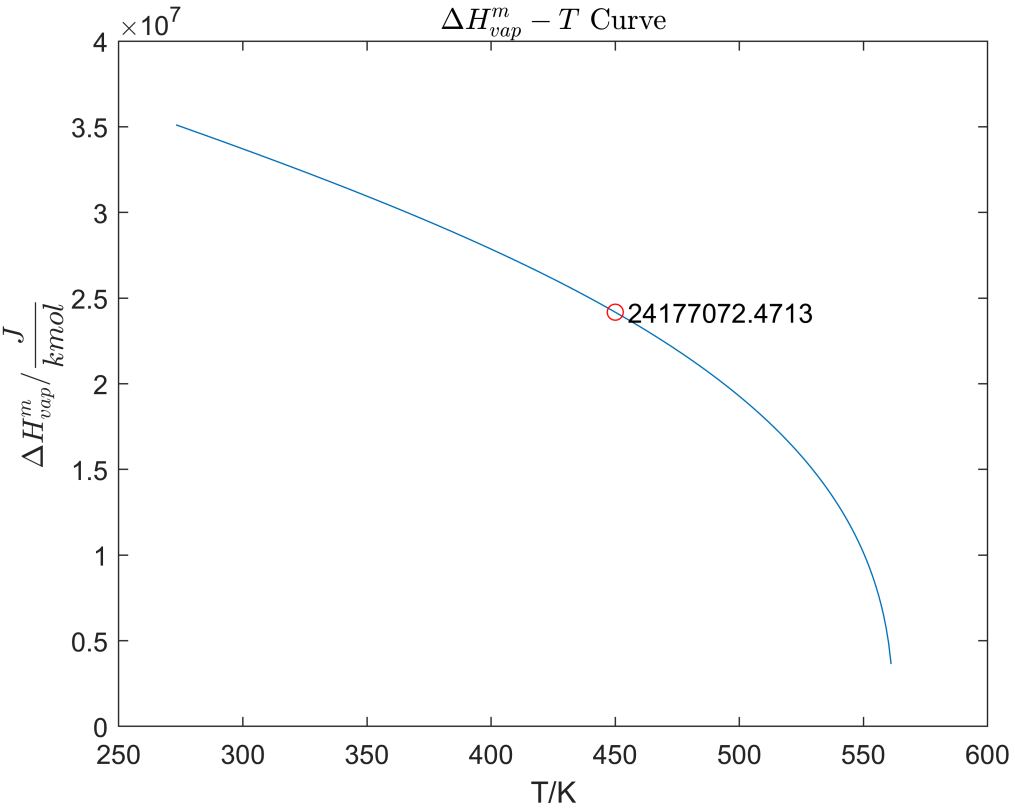
- VaporPressure, 饱和蒸汽压, Pa
- $P^* = e^{\left(A+\frac{B}{T}+C*\ln(T)+D*T^E\right)}$

```
plot([ C6H6.VaporPressure(end-1):C6H6.VaporPressure(end) ], C6H6.VaporPressure_func( [C6H6.Vapo
hold on
plot(450,  C6H6.VaporPressure_func(450), 'or')
text(455,  C6H6.VaporPressure_func(450), num2str(C6H6.VaporPressure_func(450)) )
hold off
title('$${P^*-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${ P^*/Pa }$$', 'Interpreter', 'latex')
```



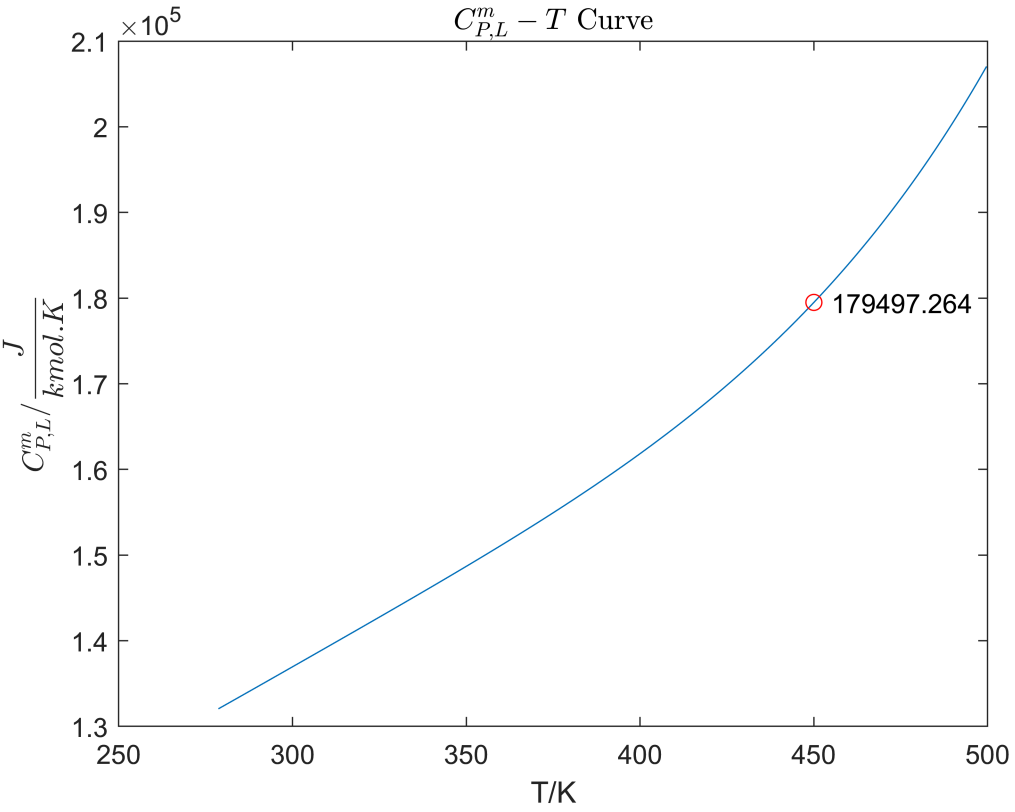
- HeatOfVaporization, 标准摩尔蒸发焓, J/kmol
- $\Delta H^m{}_{\text{vap}} = A * (1 - T_r)^{\left(B + C*T_r + D*T_r^2 + E*T_r^3\right)}, T_r = \frac{T}{\text{Tc}}$

```
plot([ C6H6.HeatOfVaporization(end-1):C6H6.HeatOfVaporization(end) ], C6H6.HeatOfVaporization_f
hold on
plot(450,  C6H6.HeatOfVaporization_func(450), 'or')
text(455,  C6H6.HeatOfVaporization_func(450), num2str(C6H6.HeatOfVaporization_func(450)) )
hold off
title('$${\Delta H^m_{vap}-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${\Delta H^m_{vap}/ \frac{J}{kmol}}$$', 'Interpreter', 'latex')
```



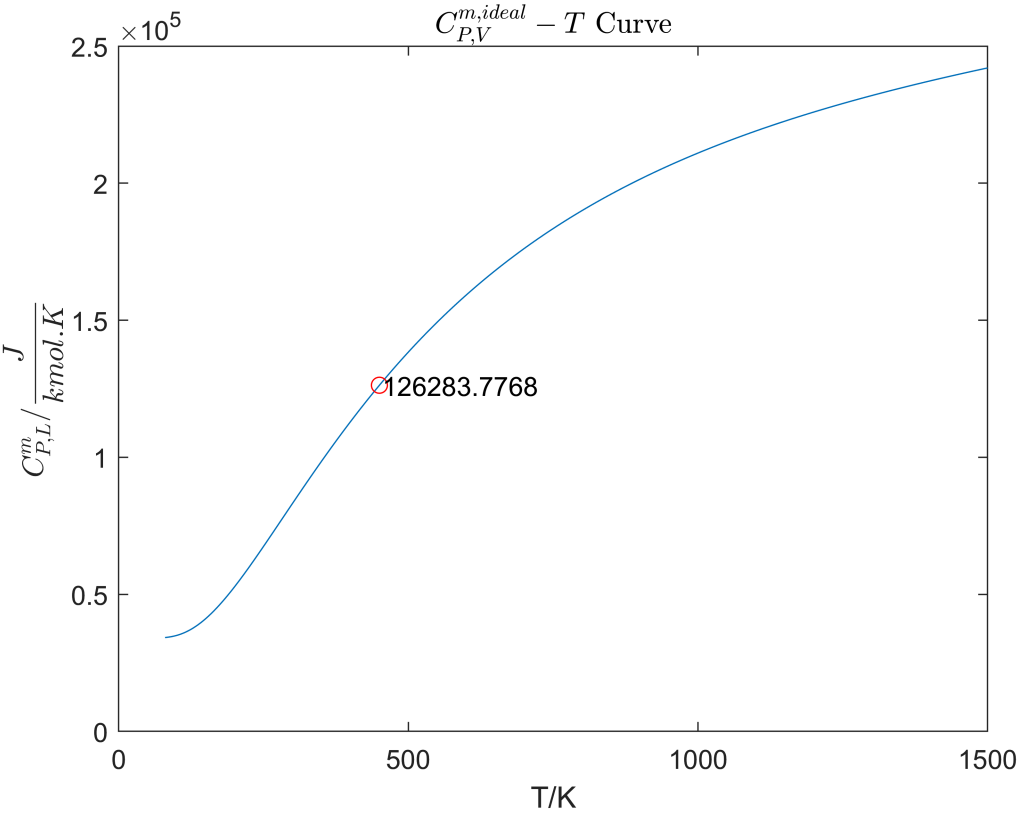
- LiquidHeatCapacityCp, 液体等压比热容, J/kmol/K
- $C_{P,L}{}^m = A + e^{\left(\frac{B}{T} + C + D*T + E*T^2\right)}$

```
plot([ C6H6.LiquidHeatCapacityCp(end-1):C6H6.LiquidHeatCapacityCp(end) ], C6H6.LiquidHeatCapaci
hold on
plot(450,  C6H6.LiquidHeatCapacityCp_func(450), 'or')
text(455,  C6H6.LiquidHeatCapacityCp_func(450), num2str(C6H6.LiquidHeatCapacityCp_func(450)) )
hold off
title('$${C^m_{P,L}-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${C^m_{P,L}/ \frac{J}{kmol.K}}$$', 'Interpreter', 'latex')
```



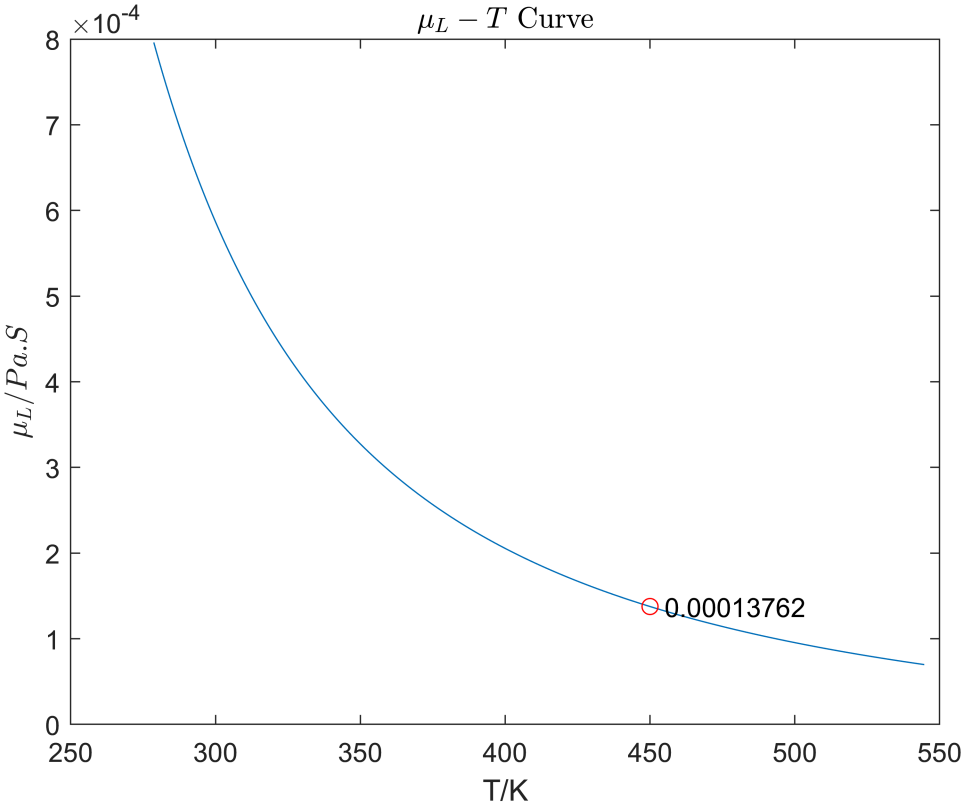
- IdealGasHeatCapacityCp, 理想气体等压比热容, J/kmol/K
- $C_{P,V}{}^{m,\text{ideal}} = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
plot([ C6H6.IdealGasHeatCapacityCp(end-1):C6H6.IdealGasHeatCapacityCp(end) ], C6H6.IdealGasHeat
hold on
plot(450,  C6H6.IdealGasHeatCapacityCp_func(450), 'or')
text(455,  C6H6.IdealGasHeatCapacityCp_func(450), num2str(C6H6.IdealGasHeatCapacityCp_func(450)
hold off
title('$${C^{m,ideal}_{P,V}-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${C^m_{P,L}/ \frac{J}{kmol.K}}$$', 'Interpreter', 'latex')
```



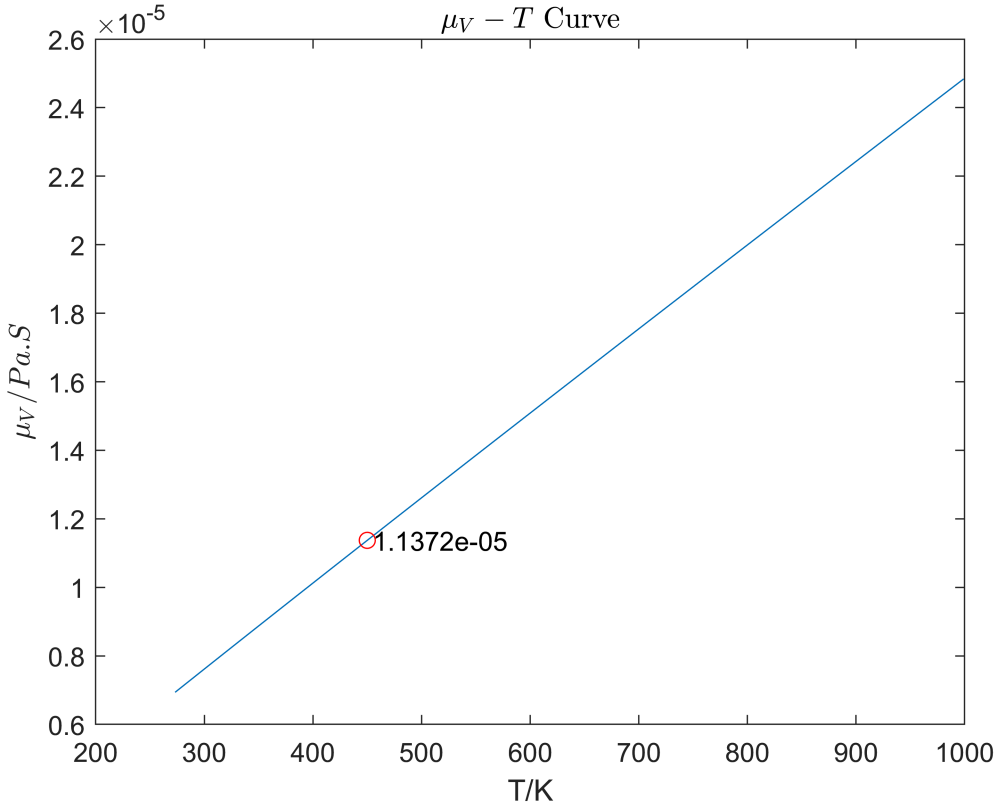
- LiquidViscosity, 液体粘度, Pa.s
- $\mu_L = e^{\left(A+\frac{B}{T}+C\ln(T)+D*T^E\right)}$

```
plot([ C6H6.LiquidViscosity(end-1):C6H6.LiquidViscosity(end) ], C6H6.LiquidViscosity_func( [ C6
hold on
plot(450,  C6H6.LiquidViscosity_func(450), 'or')
text(455,  C6H6.LiquidViscosity_func(450), num2str(C6H6.LiquidViscosity_func(450)) )
hold off
title('$${\mu_L-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${\mu_L/ Pa.S}$$', 'Interpreter', 'latex')
```



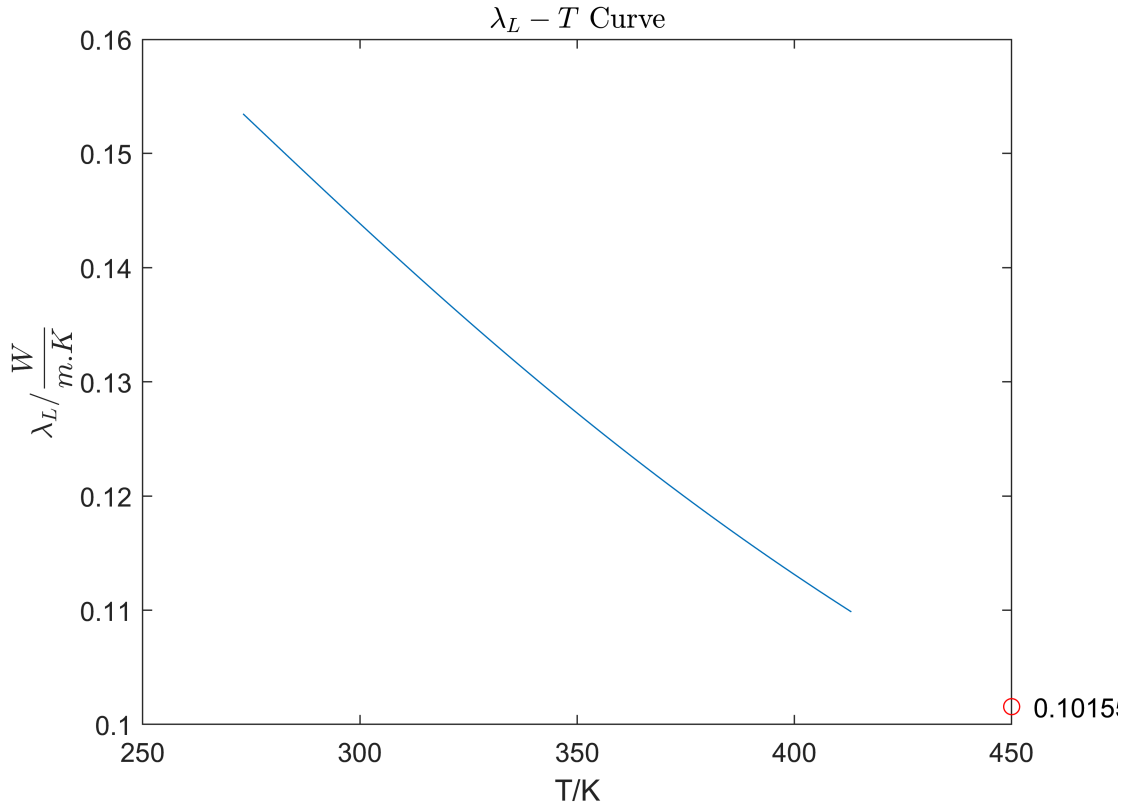
- VaporViscosity, 气体粘度, Pa.s
- $$\mu_V = \frac{A * T^B}{\left(1 + \frac{C}{T} + \frac{D}{T^2}\right)}$$

```
plot([ C6H6.VaporViscosity(end-1):C6H6.VaporViscosity(end) ], C6H6.VaporViscosity_func( [C6H6.V
hold on
plot(450,  C6H6.VaporViscosity_func(450), 'or')
text(455,  C6H6.VaporViscosity_func(450), num2str(C6H6.VaporViscosity_func(450)) )
hold off
title('$${\mu_V-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${\mu_V/ Pa.S}$$', 'Interpreter', 'latex')
```



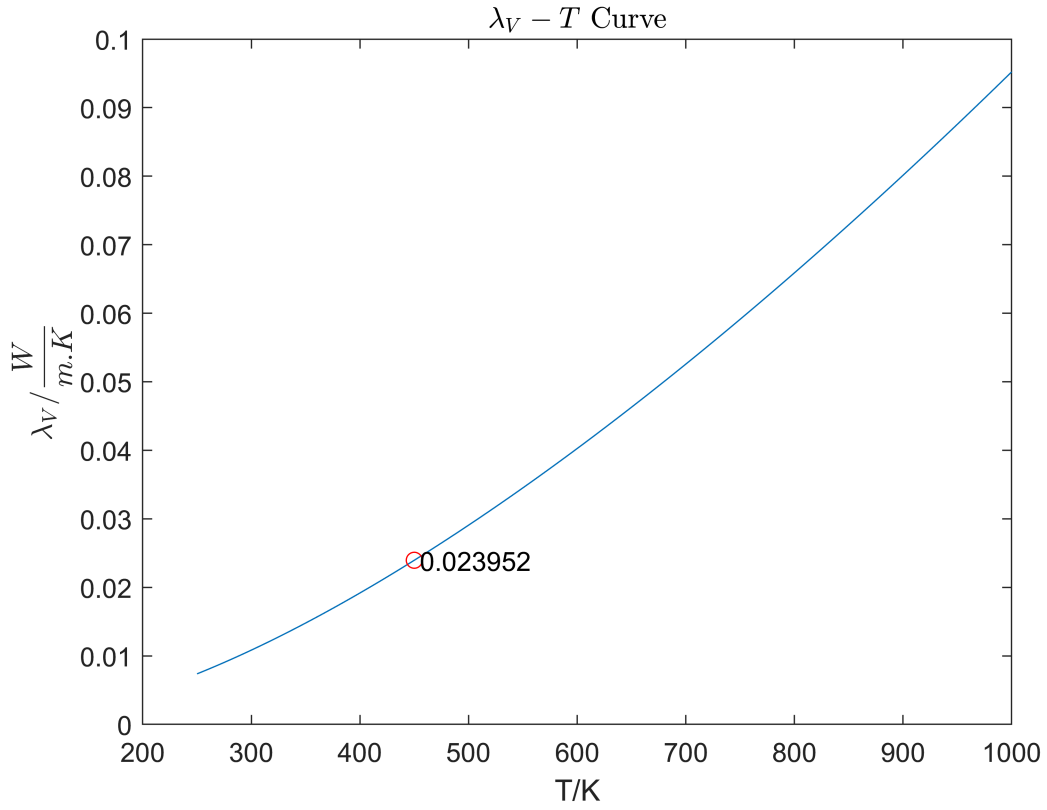
- LiquidThermalConductivity, 液体导热系数, W/m/K
- $\lambda_L = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
plot([ C6H6.LiquidThermalConductivity(end-1):C6H6.LiquidThermalConductivity(end) ], C6H6.Liquid
hold on
plot(450,  C6H6.LiquidThermalConductivity_func(450), 'or')
text(455,  C6H6.LiquidThermalConductivity_func(450), num2str(C6H6.LiquidThermalConductivity_fun
hold off
title('$${\lambda_L-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${\lambda_L/ \frac{W}{m.K}}$$', 'Interpreter', 'latex')
```



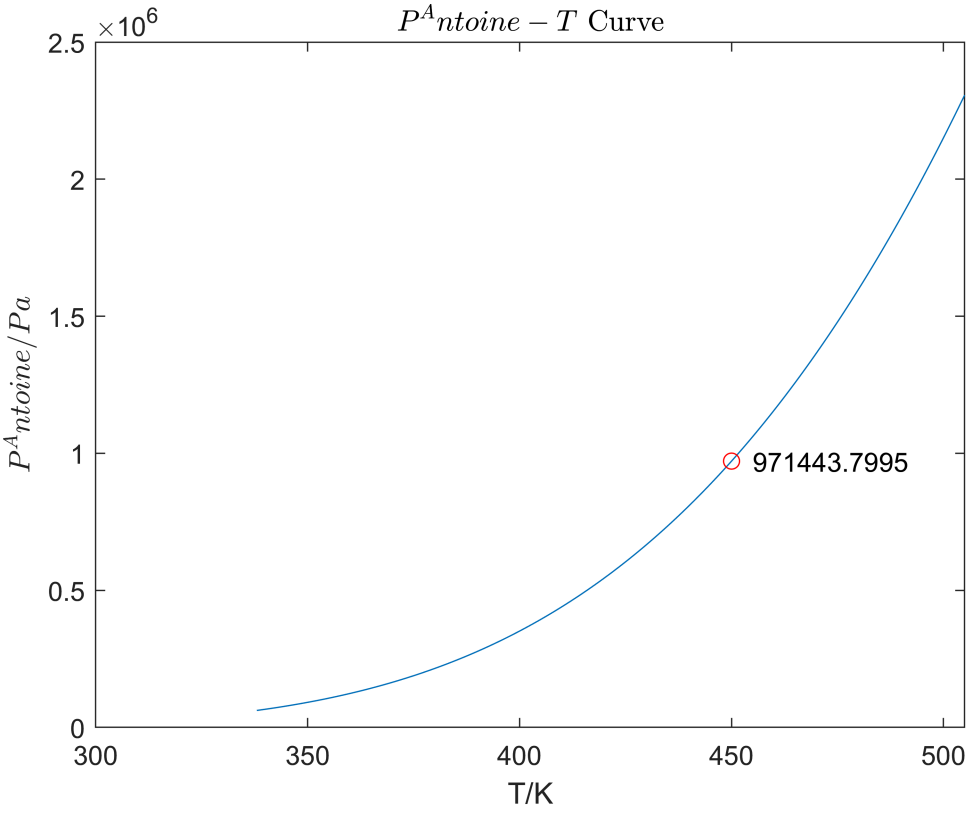
- VaporThermalConductivity, 气体导热系数, W/m/K
- $\lambda_V = \frac{A * T^B}{\left(1 + \frac{C}{T} + \frac{D}{T^2}\right)}$

```
plot([ C6H6.VaporThermalConductivity(end-1):C6H6.VaporThermalConductivity(end) ], C6H6.VaporThe
hold on
plot(450,  C6H6.VaporThermalConductivity_func(450), 'or')
text(455,  C6H6.VaporThermalConductivity_func(450), num2str(C6H6.VaporThermalConductivity_func(
hold off
title('$${\lambda_V-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${\lambda_V/ \frac{W}{m.K}}$$', 'Interpreter', 'latex')
```



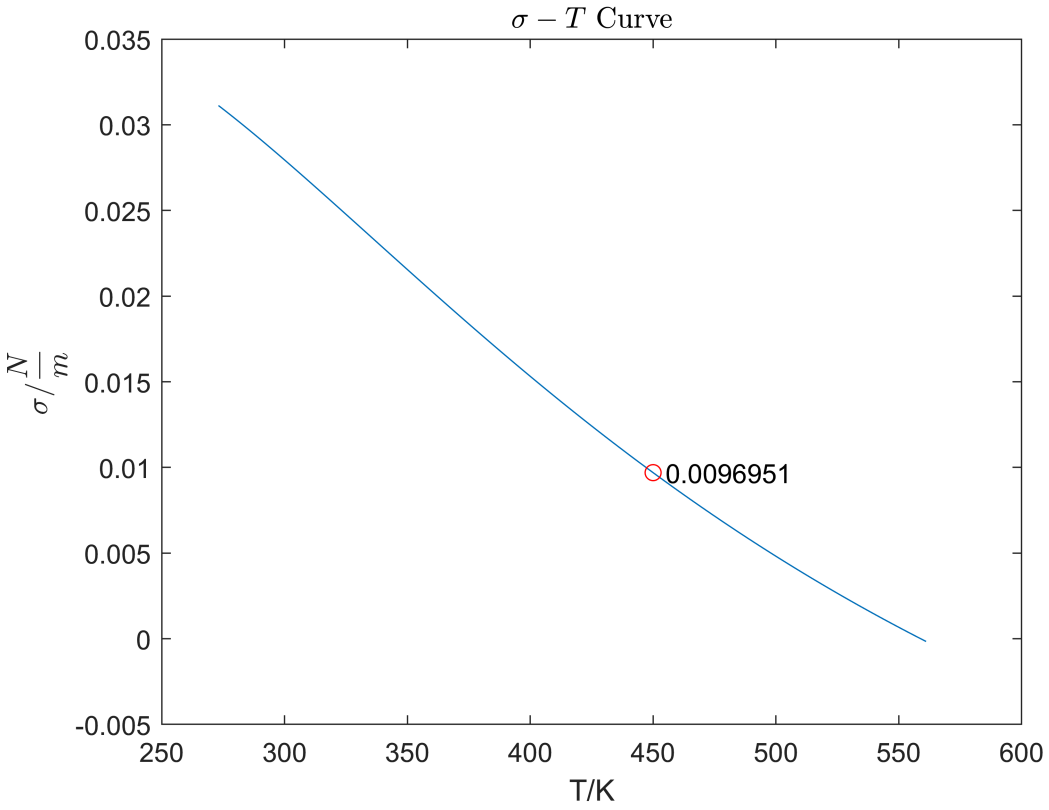
- AntoineVaporPressure, 安托因蒸汽压, Pa
- $P^{\text{Antoine}} = e^{\left(A - \frac{B}{(C+T)}\right)}$

```
plot([ C6H6.AntoineVaporPressure(end-1):C6H6.AntoineVaporPressure(end) ], C6H6.AntoineVaporPres
hold on
plot(450,  C6H6.AntoineVaporPressure_func(450), 'or')
text(455,  C6H6.AntoineVaporPressure_func(450), num2str(C6H6.AntoineVaporPressure_func(450)) )
hold off
title('$${P^Antoine-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${P^Antoine/ Pa}$$', 'Interpreter', 'latex')
```



- SurfaceTension, 表面张力, N/m
- $\sigma = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
plot([ C6H6.SurfaceTension(end-1):C6H6.SurfaceTension(end) ], C6H6.SurfaceTension_func( [C6H6.S
hold on
plot(450,  C6H6.SurfaceTension_func(450), 'or')
text(455,  C6H6.SurfaceTension_func(450), num2str(C6H6.SurfaceTension_func(450)) )
hold off
title('$${\sigma-T}$$ Curve', 'Interpreter', 'latex')
xlabel('T/K')
ylabel('$${\sigma/ \frac{N}{m}}$$', 'Interpreter', 'latex')
```




```
function Property = Component(CAS)
    CAS = [CAS, '.json'];
    PropertyParameter = jsondecode(fileread(CAS));

    Property.CAS = PropertyParameter.CAS;
    Property.Ename = PropertyParameter.CompoundID;
    Property.StructureFormula = PropertyParameter.StructureFormula;

    % Pc, 临界压力, Pa
    Property.Pc = str2double(PropertyParameter.CriticalPressure(1));
    % Tc, 临界温度, K
    Property.Tc = str2double(PropertyParameter.CriticalTemperature(1));
    % Vc, 临界体积, m3/kmol
    Property.Vc = str2double(PropertyParameter.CriticalVolume(1));
    % Zc, 临界压缩因子, -
    Property.Zc = str2double(PropertyParameter.CriticalCompressibility(1));
    % Tb, 常压沸点温度, K
    Property.Tb = str2double(PropertyParameter.NormalBoilingPointTemperature(1));
    % Ttriple, 三相点温度, K
    Property.Ttriple = str2double(PropertyParameter.TriplePointTemperature(1));
    % Ptriple, 三相点压力, Pa
    Property.Ptriple = str2double(PropertyParameter.TriplePointPressure(1));
    % Mw, 摩尔质量, kg/kmol
    Property.Mw = str2double(PropertyParameter.MolecularWeight(1));
    % Omega, 偏心因子, -
    Property.Omega = str2double(PropertyParameter.AcentricityFactor(1));
    % Hform, 标准摩尔生成焓, J/kmol
```

```
Property.Hform = str2double(PropertyParameter.HeatOfFormation(1));
% Gform, 标准摩尔生成自由能, J/kmol
Property.Gform = str2double(PropertyParameter.GibbsEnergyOfFormation(1));

% LiquidDensity, 液体的密度, kmol/m3
% LiquidDensity_func, DIPPR函数
PropertyName = 'LiquidDensity';
group = PropertyParameter.LiquidDensity(1);
equationNo = group{1}.eqno;
[Property.LiquidDensity, Property.LiquidDensity_func] = DIPPR(equationNo);

% VaporPressure, 饱和蒸汽压, Pa
% VaporPressure_func, DIPPR函数
PropertyName = 'VaporPressure';
group = PropertyParameter.VaporPressure(1);
equationNo = group{1}.eqno;
[Property.VaporPressure, Property.VaporPressure_func] = DIPPR(equationNo);

% HeatOfVaporization, 标准摩尔蒸发焓, J/kmol
% HeatOfVaporization_func, DIPPR函数
PropertyName = 'HeatOfVaporization';
group = PropertyParameter.HeatOfVaporization(1);
equationNo = group{1}.eqno;
[Property.HeatOfVaporization, Property.HeatOfVaporization_func] = DIPPR(equationNo);

% LiquidHeatCapacityCp, 液体等压比热容, J/kmol/K
% LiquidHeatCapacityCp_func, DIPPR函数
PropertyName = 'LiquidHeatCapacityCp';
group = PropertyParameter.LiquidHeatCapacityCp(1);
equationNo = group{1}.eqno;
[Property.LiquidHeatCapacityCp, Property.LiquidHeatCapacityCp_func] = DIPPR(equationNo);

% IdealGasHeatCapacityCp, 理想气体等压比热容, J/kmol/K
% IdealGasHeatCapacityCp_func, DIPPR函数
PropertyName = 'IdealGasHeatCapacityCp';
group = PropertyParameter.IdealGasHeatCapacityCp(1);
equationNo = group{1}.eqno;
[Property.IdealGasHeatCapacityCp, Property.IdealGasHeatCapacityCp_func] = DIPPR(equationNo)

% LiquidViscosity, 液体粘度, Pa.s
% LiquidViscosity, DIPPR函数
PropertyName = 'LiquidViscosity';
group = PropertyParameter.LiquidViscosity(1);
equationNo = group{1}.eqno;
[Property.LiquidViscosity, Property.LiquidViscosity_func] = DIPPR(equationNo);

% VaporViscosity, 气体粘度, Pa.s
% VaporViscosity_func, DIPPR函数
PropertyName = 'VaporViscosity';
group = PropertyParameter.VaporViscosity(1);
equationNo = group{1}.eqno;
[Property.VaporViscosity, Property.VaporViscosity_func] = DIPPR(equationNo);

% LiquidThermalConductivity, 液体导热系数, W/m/K
```

```
% LiquidThermalConductivity_func, DIPPR函数
PropertyName = 'LiquidThermalConductivity';
group = PropertyParameter.LiquidThermalConductivity(1);
equationNo = group{1}.eqno;
[Property.LiquidThermalConductivity, Property.LiquidThermalConductivity_func] = DIPPR(equat

% VaporThermalConductivity, 气体导热系数, W/m/K
% VaporThermalConductivity_func, DIPPR函数
PropertyName = 'VaporThermalConductivity';
group = PropertyParameter.VaporThermalConductivity(1);
equationNo = group{1}.eqno;
[Property.VaporThermalConductivity, Property.VaporThermalConductivity_func] = DIPPR(equatio

% AntoineVaporPressure, 安托因蒸汽压, Pa
% AntoineVaporPressure_func, DIPPR函数
PropertyName = 'AntoineVaporPressure';
group = PropertyParameter.AntoineVaporPressure(1);
equationNo = group{1}.eqno;
[Property.AntoineVaporPressure, Property.AntoineVaporPressure_func] = DIPPR(equationNo);


% SurfaceTension, 表面张力, N/m
% SurfaceTension_func, DIPPR函数
PropertyName = 'SurfaceTension';
group = PropertyParameter.SurfaceTension(1);
equationNo = group{1}.eqno;
[Property.SurfaceTension, Property.SurfaceTension_func] = DIPPR(equationNo);

function [para, func] = DIPPR(equationNo)
    equation = PropertyParameter.(PropertyName)(1);
    Tmin = str2double(equation{1}.Tmin);
    Tmax = str2double(equation{1}.Tmax);
    switch equationNo
        case '1'
            A = str2double(equation{1}.A);
            para = [A,Tmin,Tmax];
            func = @(T) A;
        case '2'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            para = [A,B,Tmin,Tmax];
            func = @(T) A + B.*T;
        case '3'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            para = [A,B,C,Tmin,Tmax];
            func = @(T) A + B.*T + C.*T.^2;
        case '4'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            para = [A,B,C,D,Tmin,Tmax];
```

```
            func = @(T) A + B.*T + C.*T.^2 + D.*T.^3;
        case '5'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A + B.*T + C.*T.^2 + D.*T.^3 + E.*T.^4;
        case '6'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A + B.*T + C.*T.^2 + D.*T.^3 + E./T.^2;
        case '10'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            para = [A,B,C,Tmin,Tmax];
            func = @(T) exp(A - B./(C+T));
        case '16'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A + exp(B./T + C + D*T + E.*T.^2);
        case '100'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A + B.*T + C.*T.^2 + D.*T.^3 + E.*T.^4;
        case '101'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) exp(A + B./T + C.*log(T) + D.*T.^E);
        case '102'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            para = [A,B,C,D,Tmin,Tmax];
            func = @(T) A.*T.^B./(1 + C./T + D./T.^2);
```

```
        case '103'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            para = [A,B,C,D,Tmin,Tmax];
            func = @(T) A + B.*exp(-C./T.^D);
        case '104'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A + B./T + C*10^6./T.^3 + D*10^16./T.^8 + E*10^18./T.^9;
        case '105'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            para = [A,B,C,D,Tmin,Tmax];
            func = @(T) A./B.^(1+(1-T/C).^D);
        case '106'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A.*(1-T./Property.Tc).^(B + C.*(T./Property.Tc) + D.*(T./Property.T
        case '107'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A + B.*(C./T./sinh(C./T)).^2 + E.*(D./T./cosh(D./T)).^2;
        case '114'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            para = [A,B,C,D,Tmin,Tmax];
            func = @(T) A.*T + B.*T.^2/2 + C.*T.^3/3 + D.*T.^4/4;
        case '117'
            A = str2double(equation{1}.A);
            B = str2double(equation{1}.B);
            C = str2double(equation{1}.C);
            D = str2double(equation{1}.D);
            E = str2double(equation{1}.E);
            para = [A,B,C,D,E,Tmin,Tmax];
            func = @(T) A.*T + B.*(C./T)./tanh(C./T) - D.*(E./T)./tanh(E./T);
    end
```

```
    end

end
```