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 =
     5.620500000000000e+02
```

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

```
Vc = C6H6.Vc
```

```
Vc =
   0.256000000000000
```

- Zc, 临界压缩因子, -

```
Zc = C6H6.Zc
```

```
Zc =
   0.268000000000000
```

- Tb, 常压沸点温度, K

```
Tb = C6H6.Tb
```

```
Tb =
     3.532400000000000e+02
```

- Ttriple, 三相点温度, K

```
Ttriple = C6H6.Ttriple
```

```
Ttriple =
     2.786800000000000e+02
```

- Ptriple, 三相点压力, Pa

```
Ptriple = C6H6.Ptriple
```

```
Ptriple =
     4.764220000000000e+03
```

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

```
Mw = C6H6.Mw
```

```
Mw =
  78.114000000000004
```

- ω，偏心因子, -

```
omega = C6H6.omega
```

```
omega =
   0.209000000000000
```

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

```
Hfrom = C6H6.Hform
```

```
Hfrom =
    82880000
```

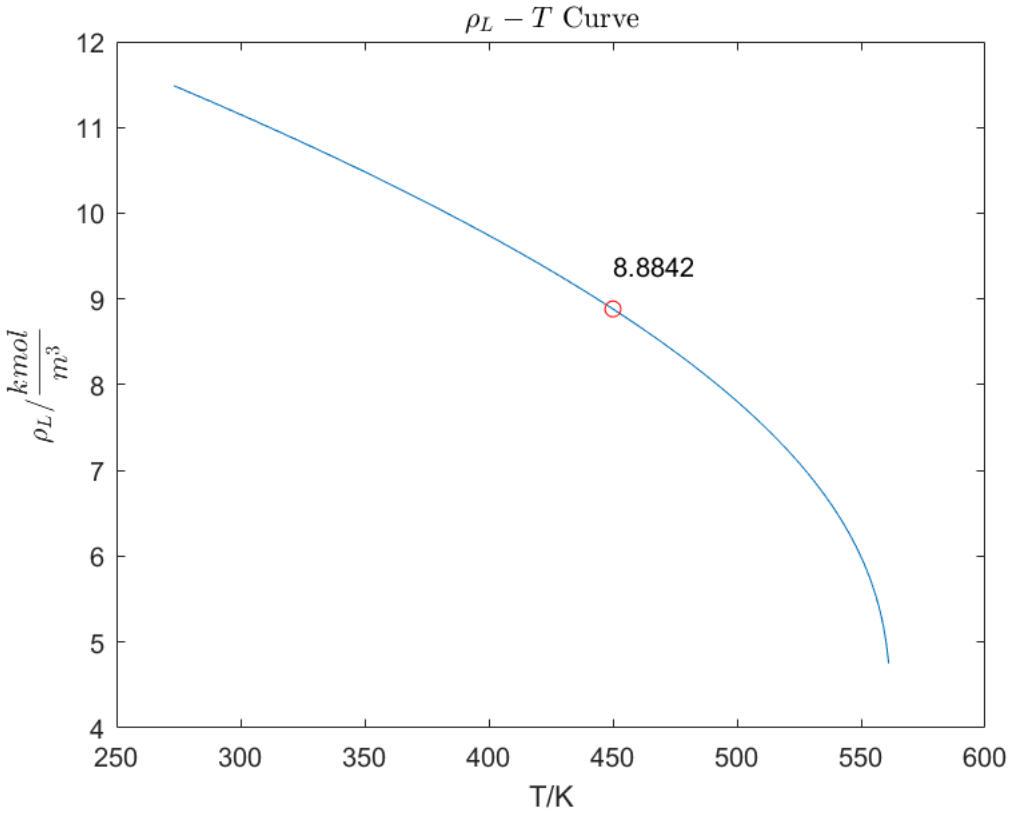
- G^{m}_{fron}，标准摩尔生成自由能, $\frac{J}{\text{kmol}}$

```
Gform = C6H6.Gform
```

```
Gform =
   129600000
```

- LiquidDensity, 液体的密度, kmol/m^3
- $\rho_L = \frac{A}{B^{\left(1+\left(1-\frac{T}{C}\right)^{D}\right)}}$

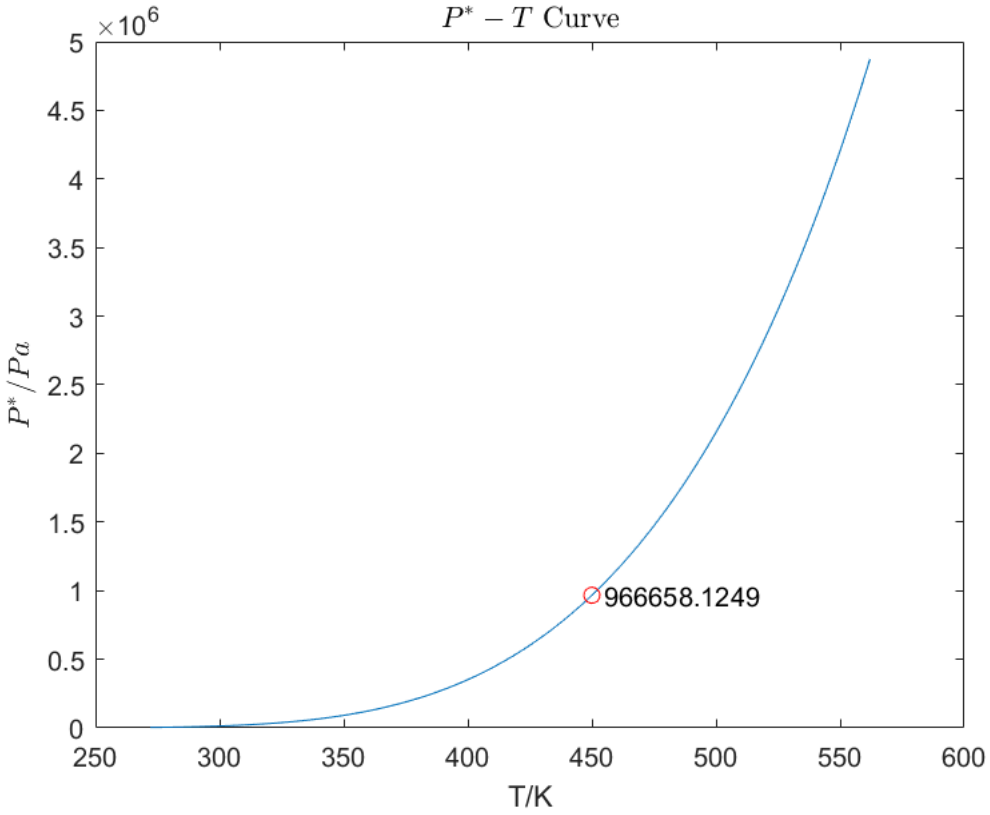
```
plot([ C6H6.LiquidDensity(end-1):C6H6.LiquidDensity(end) ], C6H6.LiquidDensity_func( [C6H6.Liqu
hold on
plot(450,  C6H6.LiquidDensity_func(450), 'or')
text(450,  C6H6.LiquidDensity_func(450)+0.5, num2str(C6H6.LiquidDensity_func(450)) )
hold off
title('$${\rho_L-T}$$ Curve', 'Interpreter', 'latex')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



- VaporPressure, 饱和蒸汽压, Pa

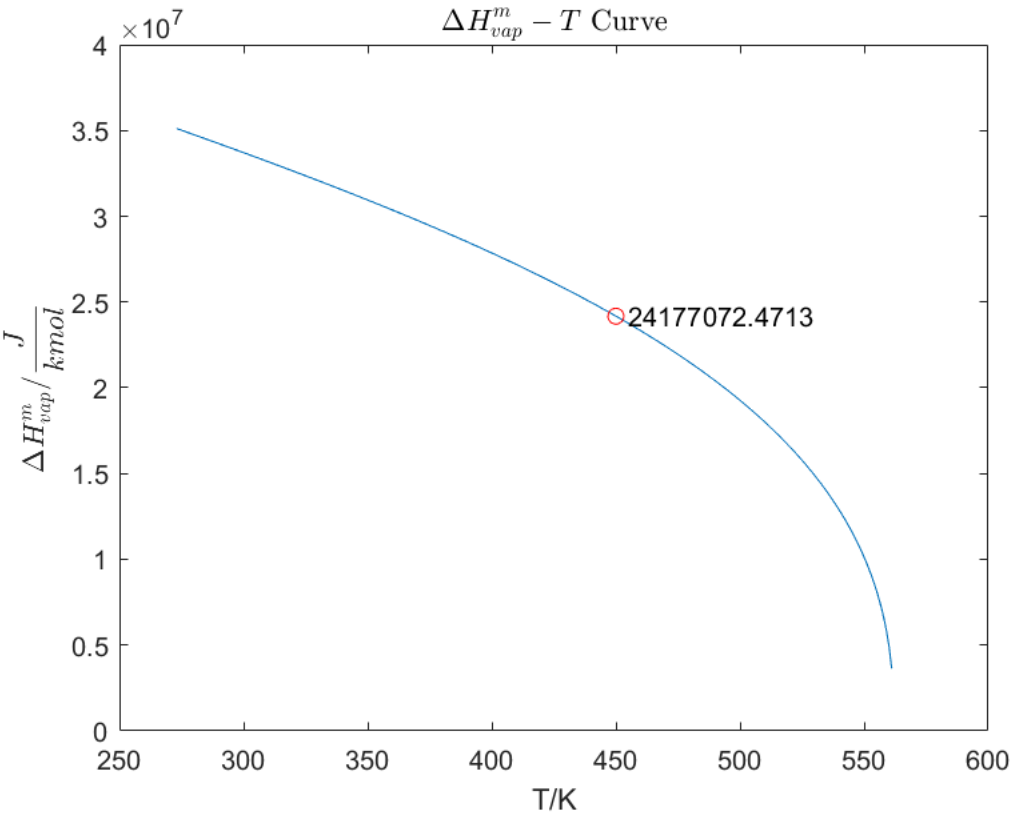
- $P^* = e^{\left(A+\frac{B}{T}+C*\ln(T)+D*T^E\right)}$

```
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')
```



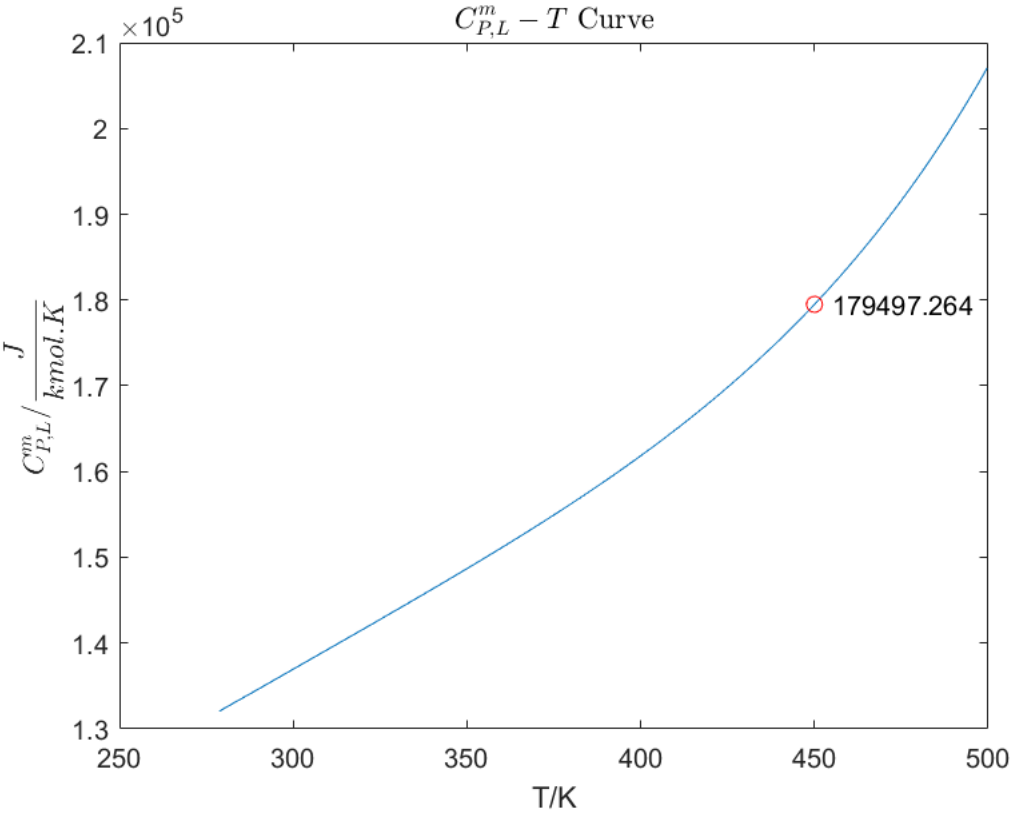
- HeatOfVaporization, 标准摩尔蒸发焓, J/kmol
- $\Delta H^m{}_{\text{vap}} = A * (1 - T_r)^{\left(B+C*T_r+D*T_r^2+E*T_r^3\right)}, T_r = \frac{T}{\text{Tc}}$

```
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')
```



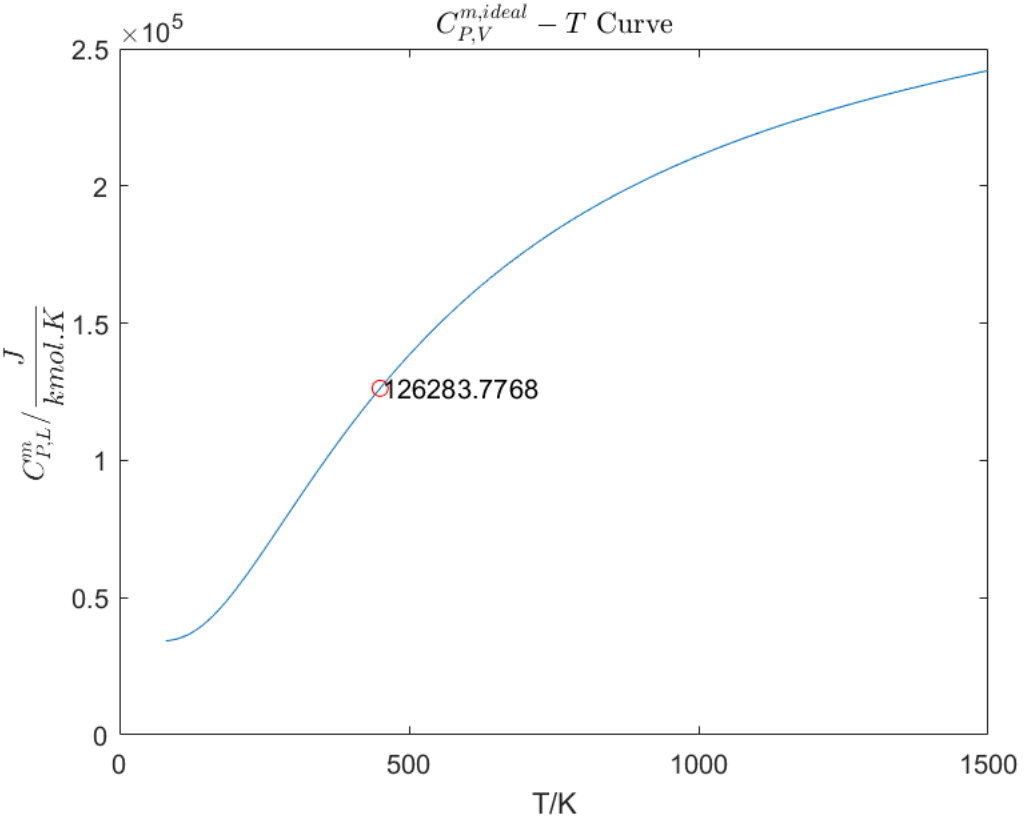
- LiquidHeatCapacityCp, 液体等压比热容, J/kmol/K
- $C_{P,L}{}^{m} = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
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')
```



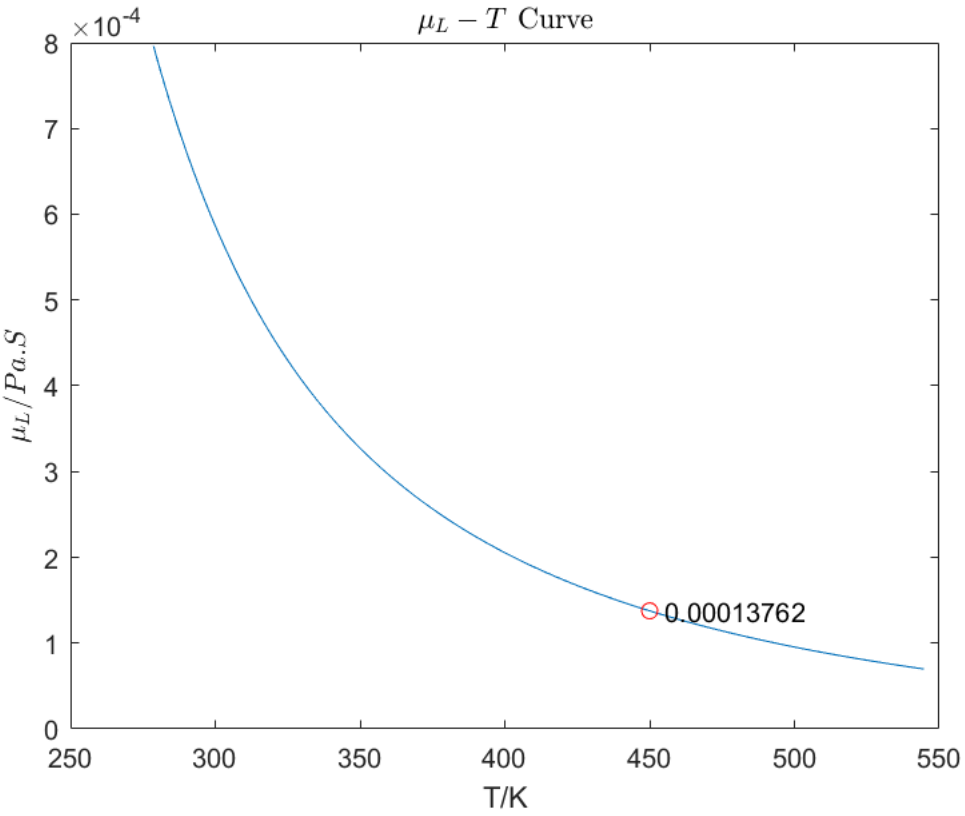
- IdealGasHeatCapacityCp, 理想气体等压比热容, J/kmol/K
- $C_{P,V}{}^{m,\text{ideal}} = A + e^{\left(\frac{B}{T} + C + D*T + E*T^2\right)}$

```
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')
```



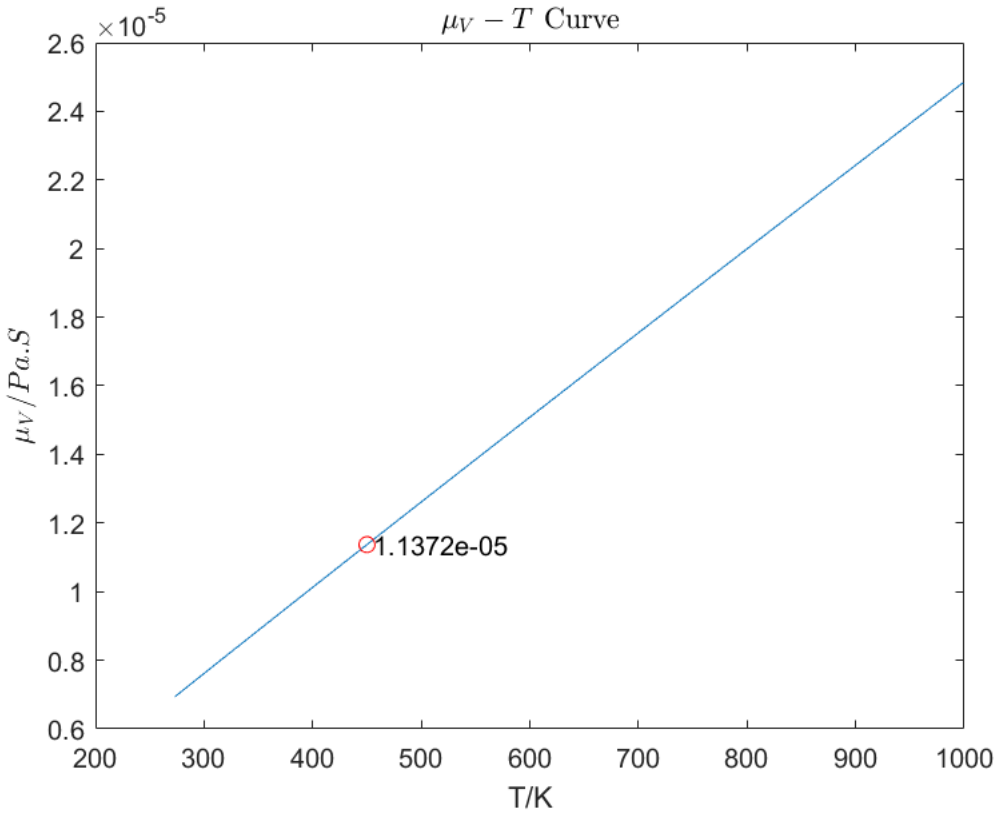
- LiquidViscosity, 液体粘度, Pa.s
- $\mu_L = e^{\left(A+\frac{B}{T}+C\ln(T)+D*T^E\right)}$

```
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')
```



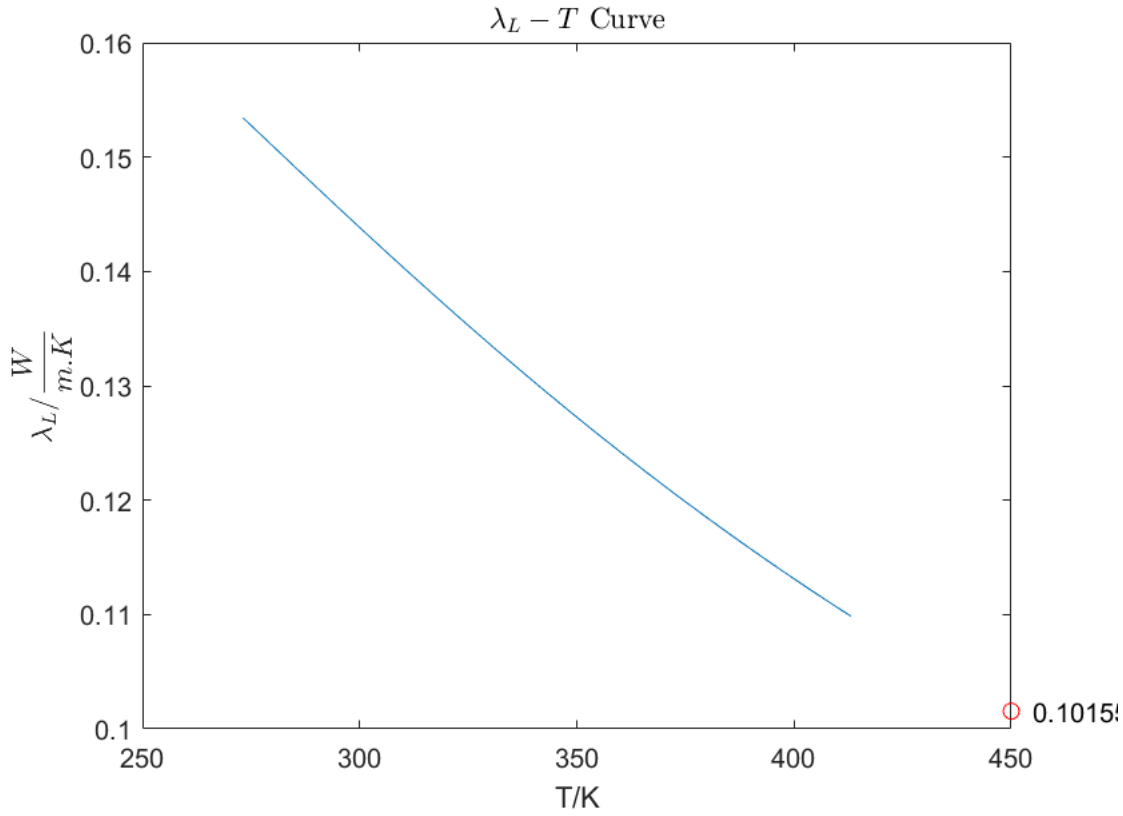
- VaporViscosity, 气体粘度, Pa.s
- $$\mu_V = \frac{A * T^B}{\left(1 + \frac{C}{T} + \frac{D}{T^2}\right)}$$

```
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')
```



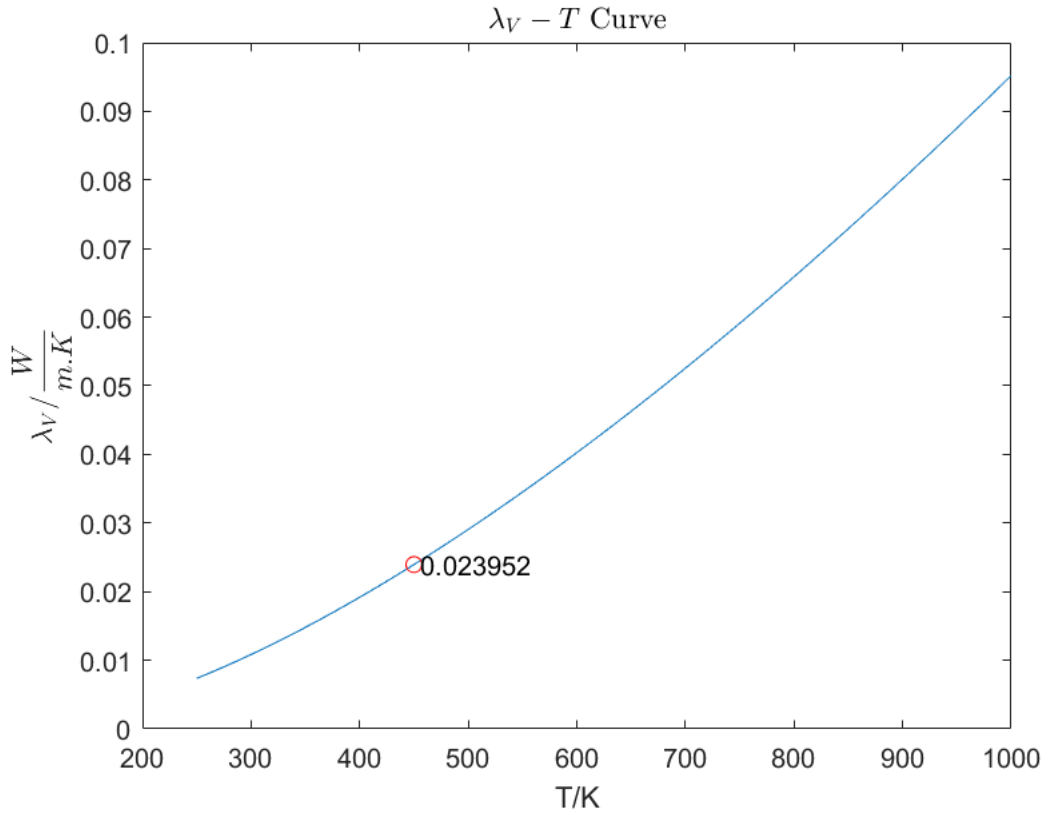
- LiquidThermalConductivity, 液体导热系数, W/m/K
- $\lambda_L = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
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')
```



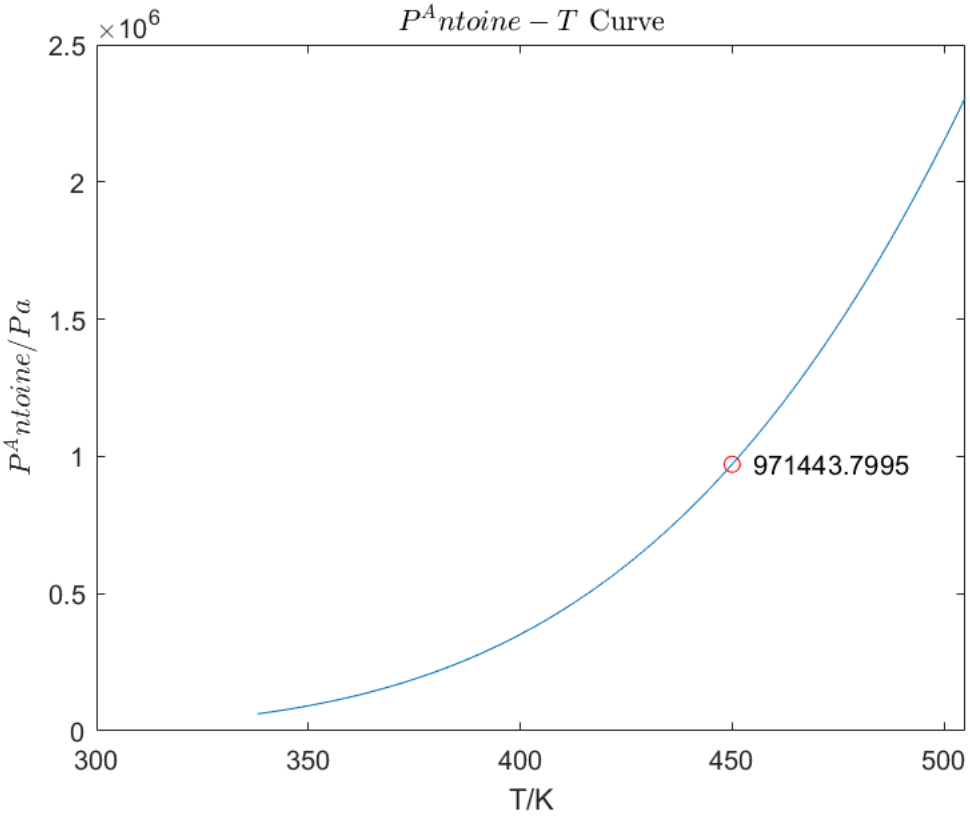
- VaporThermalConductivity, 气体导热系数, W/m/K
- $\lambda_V = \frac{A * T^B}{\left(1 + \frac{C}{T} + \frac{D}{T^2}\right)}$

```
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')
```



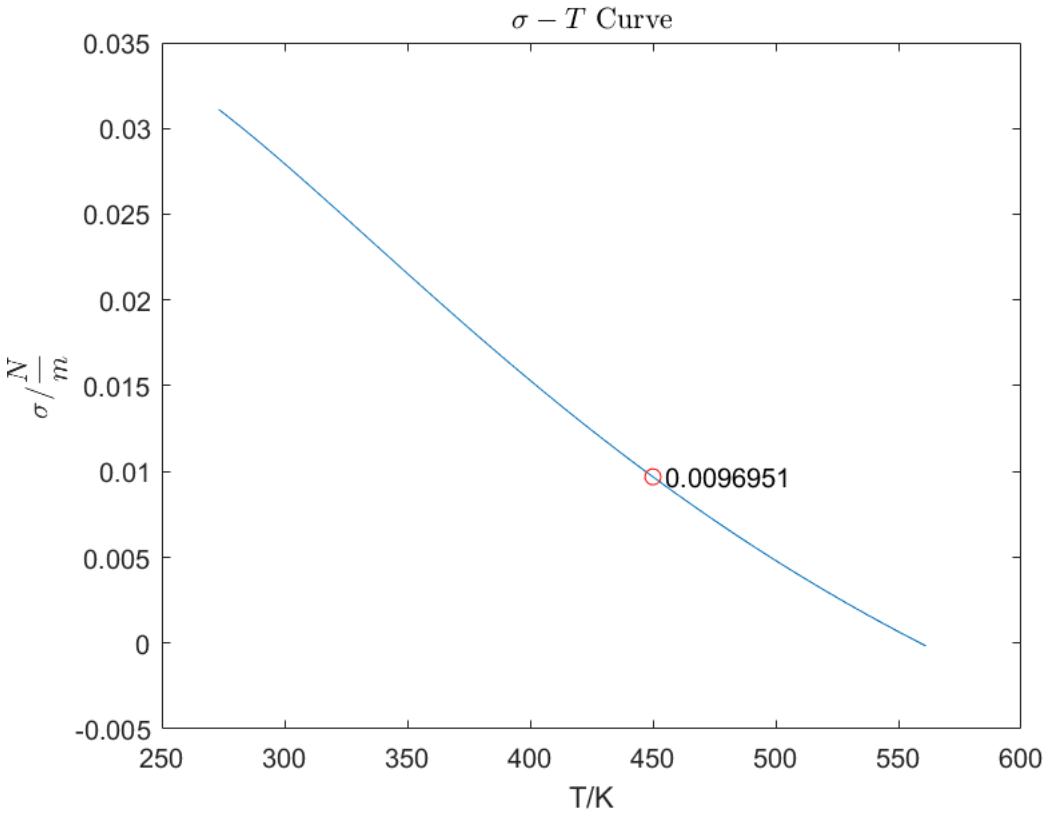
- AntoineVaporPressure, 安托因蒸汽压, Pa
- $P^{\text{Antoine}} = e^{\left(A - \frac{B}{(C+T)}\right)}$

```
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')
```



纯物质,丙烷为例,计算体积

```
CAS = '74-98-6';
Propane = Component(CAS);
P = 997420;
T = 300;
z = 1;
q = 1;
Zl = EOS(P,T,z,q,Propane);
Vl = Zl*8.314*T/P
```

```
Vl =
     8.676502462792916e-05
```

```
q = 0;
Zv = EOS(P,T,z,q,Propane);
Vv = Zv*8.314*T/P
```

```
Vv =
   0.002038518631244
```

```
P = 4247700;
T =369.85;
q = 0;
Zcritical = EOS(P,T,z,q,Propane);
Vcritical = Zcritical*8.314*T/P
```

```
Vcritical =
     2.414393810261508e-04
```

```
R12 = Propane;
R22 = Propane;
R12.Pc = 4.224*10^6;
R12.Tc = 385;
R12.omega = 0.176;
R22.Pc = 4.975*10^6;
R22.Tc = 369.2;
R22.omega = 0.215;
P = 1.0*10^6;
T = 400;
q = 0;
z = [0.5,0.5];
for P = [1:5]*10^6
    Zv = EOS(P,T,z,q,[R22,R12])
    Vv = Zv*8.314*T/P
end
```

```
Zv =
   0.928653697117342
Vv =
   0.003088330735133
Zv =
   0.852546345387205
Vv =
   0.001417614063110
Zv =
   0.769907552167168
Vv =
   8.534681851623783e-04
Zv =
   0.677720872158938
Vv =
   5.634571331129412e-04
Zv =
   0.570682190200430
Vv =
   3.795721383461101e-04
```

混合物,R12(CCl2F2)和R22(CHClF2为例,计算体积

```
R12 = Propane;
R22 = Propane;
R12.Pc = 4.224*10^6;
R12.Tc = 385;
R12.omega = 0.176;
R22.Pc = 4.975*10^6;
R22.Tc = 369.2;
R22.omega = 0.215;
P = 1.0*10^6;
T = 400;
q = 0;
z = [0.5,0.5];
for P = [1:5]*10^6
    Zv = EOS(P,T,z,q,[R22,R12])
    Vv = Zv*8.314*T/P
end
```

```
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

function Z = EOS(P,T,z,q,Component)
    % Constant;
    R = 8.314;
    c = length(z);
    z = z./sum(z);
    Pc = ones(c,1);
    Tc = ones(c,1);
    omega = ones(c,1);
    Mw = ones(c,1);
    for i = 1:c
        Pc(i) = Component(i).Pc;
        Tc(i) = Component(i).Tc;
        omega(i) = Component(i).omega;
        Mw(i) = Component(i).Mw;
    end

    % PR 方程系数
```

```
    Omega_a = 0.45724;
    Omega_b = 0.0778;
    m = [0.37464, 1.54226, -0.2699];

    alpha = (1+ (m(1) + m(2).*omega + m(3).*omega.^2).*(1-(T./Tc).^0.5) ).^2;
    a_i = Omega_a.*R.^2.*Tc.^2./Pc .* alpha;
    b_i = Omega_b*R.*Tc./Pc;
    a = MixRule(z,a_i,0,2);
    b = MixRule(z,b_i,0,1);

    % PR 方程关系式
    B = b*P/R/T;
    delta = 2*B;
    varepsilon = -B^2;
    eta = B;
    A = a*P/(R*T)^2;

    EOS_coeff = [1, delta-B-1, A+varepsilon-delta*(B+1), -(varepsilon*(B+1)+A*eta)];
    Z = roots(EOS_coeff);
    Z = Z(imag(Z) == 0);

    % q, 液相分率, [0,1]
    if q == 1
        Z = min(Z);
    elseif q == 0
        Z = max(Z);
    end

    function Q = MixRule(z,Q_i,kij,rule)
        % z, 为摩尔组成, 1*c
        % Q_i, 为物性参数量, c*1
        % rule, 混合规则
        % kij, 二元交互参数, c*c
        % 一般情况下, 默认i=j时, kij = 0;
        if nargin == 3
            kij = 0;
        end

        switch rule
            case 1
                Q = z*Q_i;
            case 2
                Q = z*( (Q_i*Q_i').^0.5 ).*(1-kij)*z';
        end

    end

end
```