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, $\frac{J}{\mathrm{kmol}}$

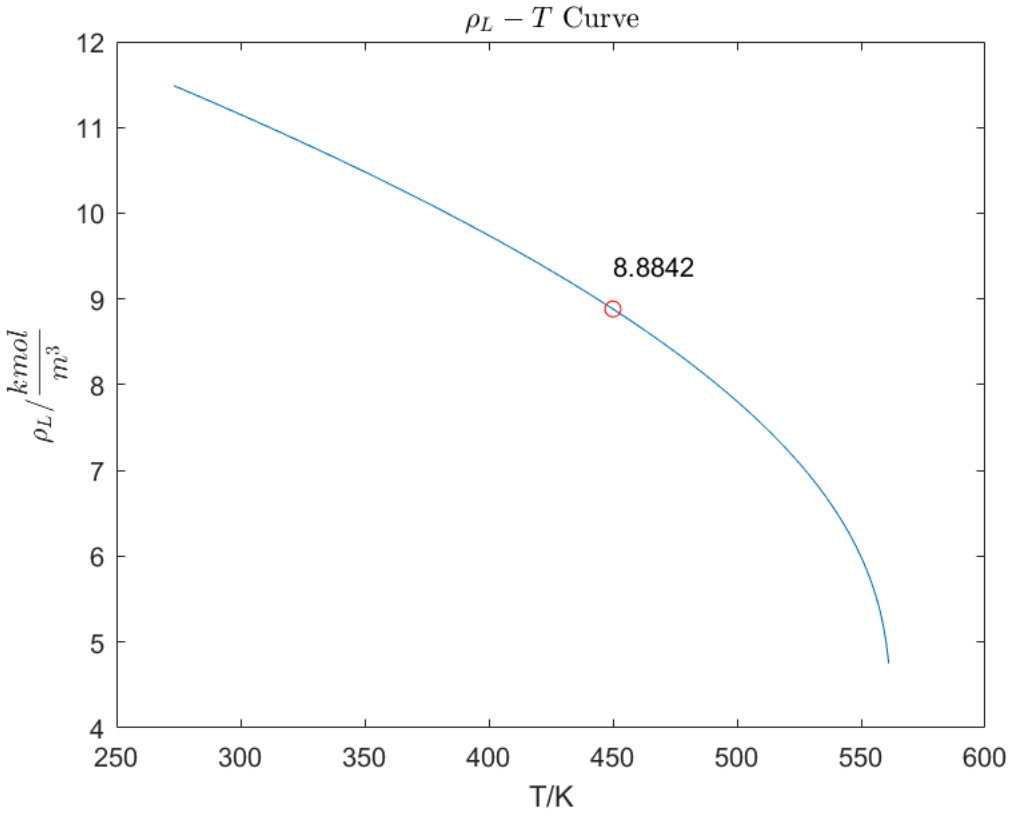
```
Gform = C6H6.Gform
```

```
Gform = 129600000
```

- LiquidDensity, 液体的密度, kmol/m^3

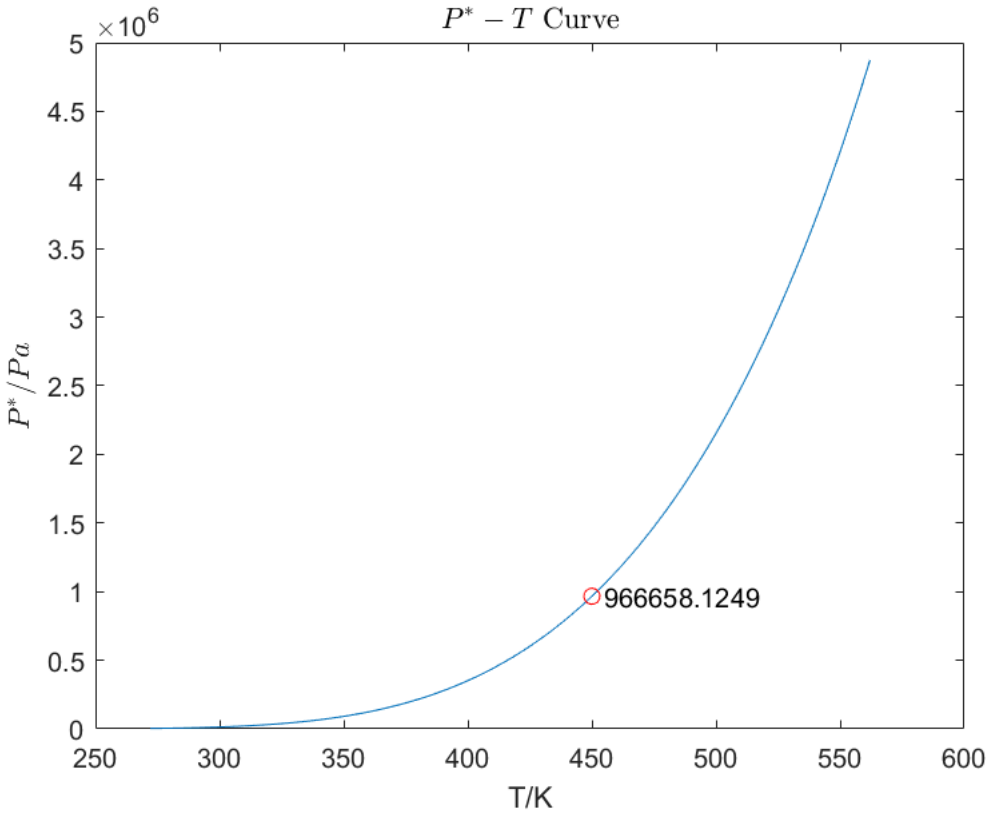
- $\rho_L = \frac{A}{B^{\left(1+\left(1-\frac{T}{C}\right)^{D}\right)}}$

```
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')
```



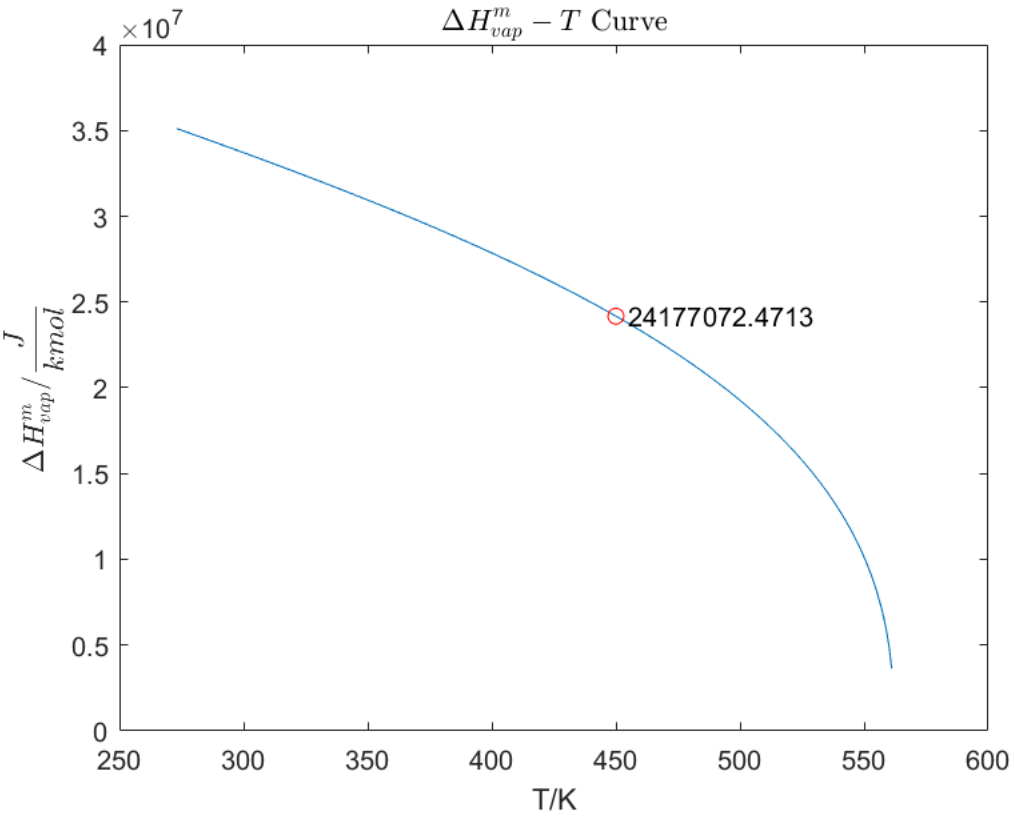
- VaporPressure, 饱和蒸汽压, Pa
- $P^* = e^{\left(A+\frac{B}{T}+C*\ln(T)+D*T^E\right)}$

```
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')
```



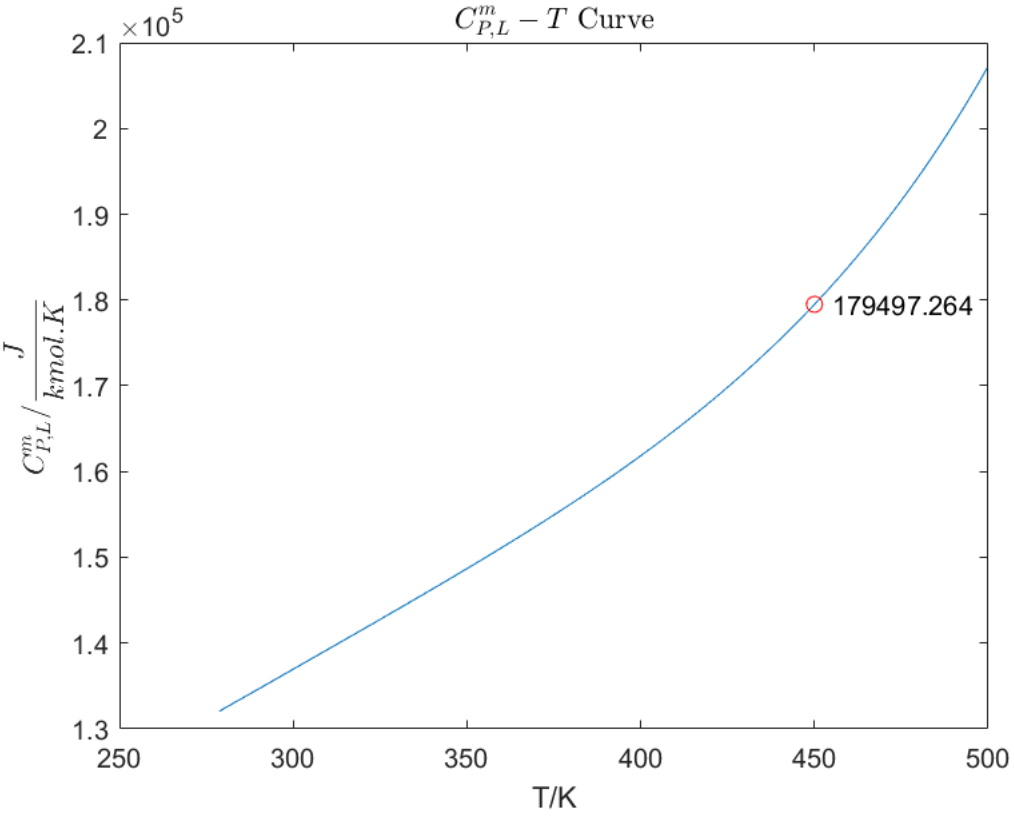
- HeatOfVaporization, 标准摩尔蒸发焓, J/kmol
- $\Delta H^m{}_{\text{vap}} = A * (1 - T_r)^{\left(B + C*T_r + D*T_r^2 + E*T_r^3\right)}, T_r = \frac{T}{\text{Tc}}$

```
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')
```



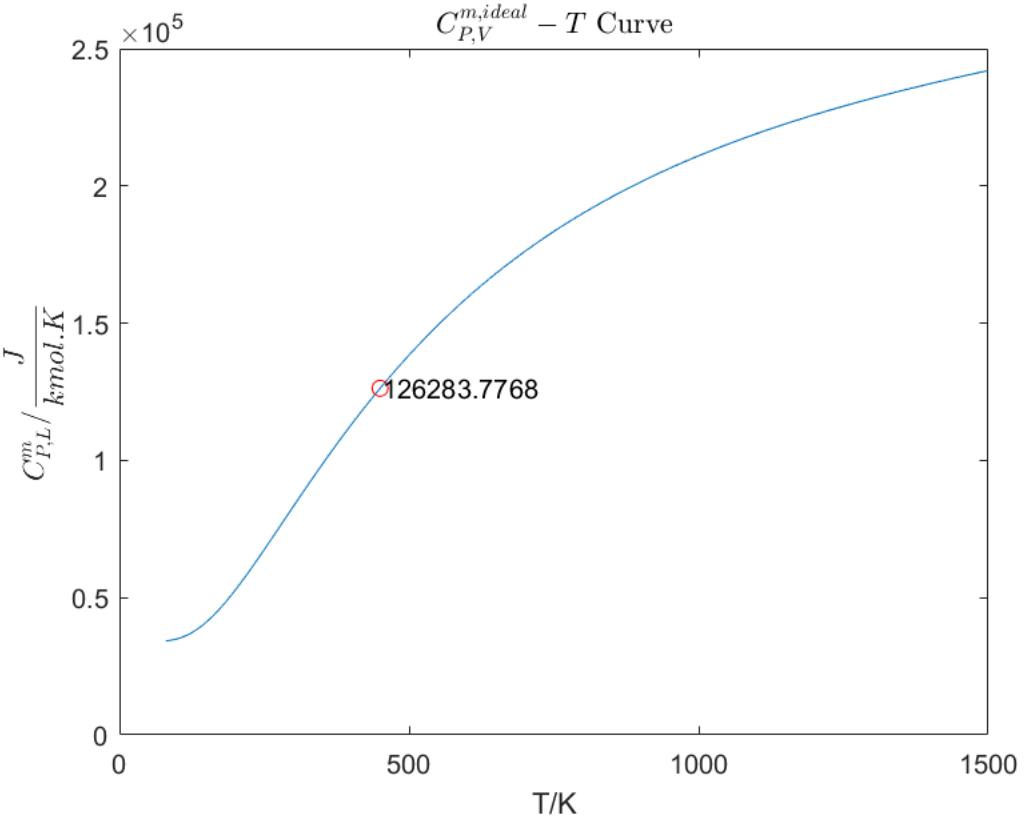
- LiquidHeatCapacityCp, 液体等压比热容, J/kmol/K
- $C_{P,L}{}^{m} = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
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')
```



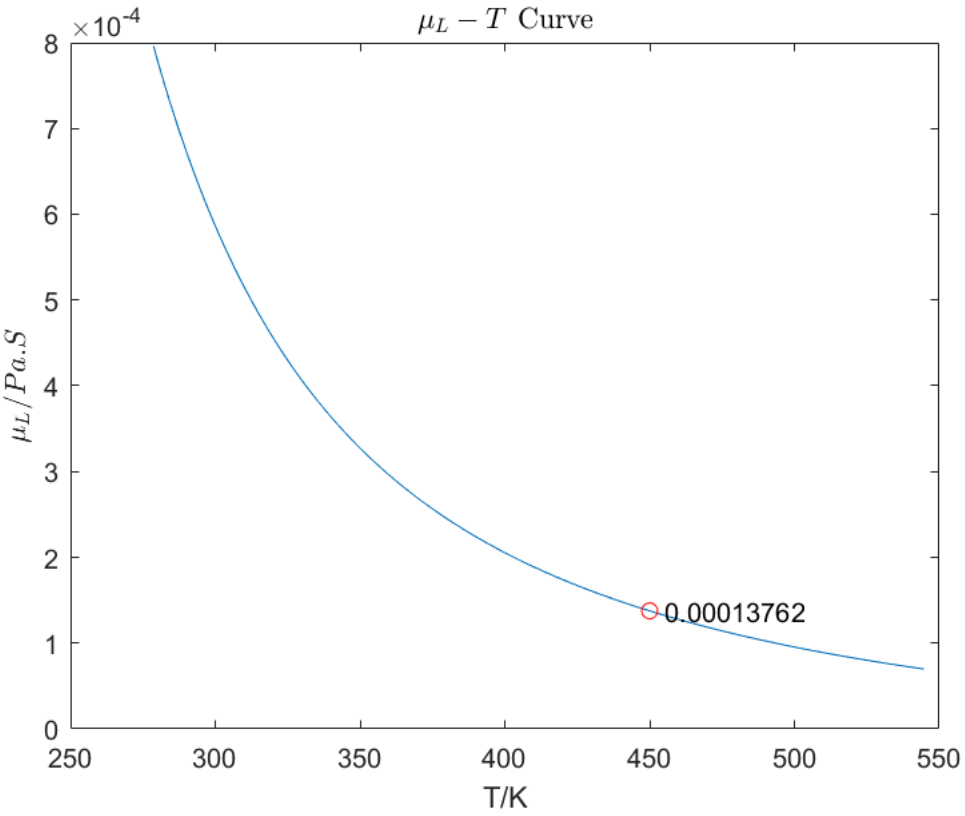
- IdealGasHeatCapacityCp, 理想气体等压比热容, J/kmol/K
- $C_{P,V}{}^{m,\text{ideal}} = A + e^{\left(\frac{B}{T} + C + D*T + E*T^2\right)}$

```
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')
```



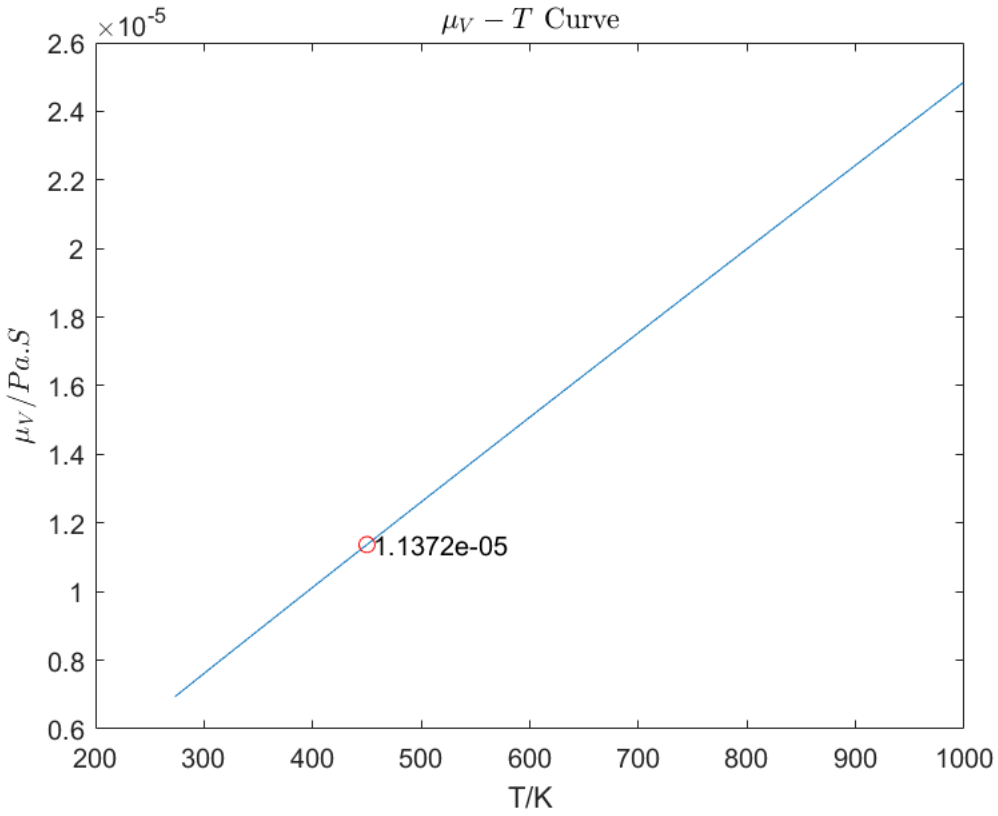
- LiquidViscosity, 液体粘度, Pa.s
- $\mu_L = e^{\left(A+\frac{B}{T}+C\ln(T)+D*T^E\right)}$

```
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')
```



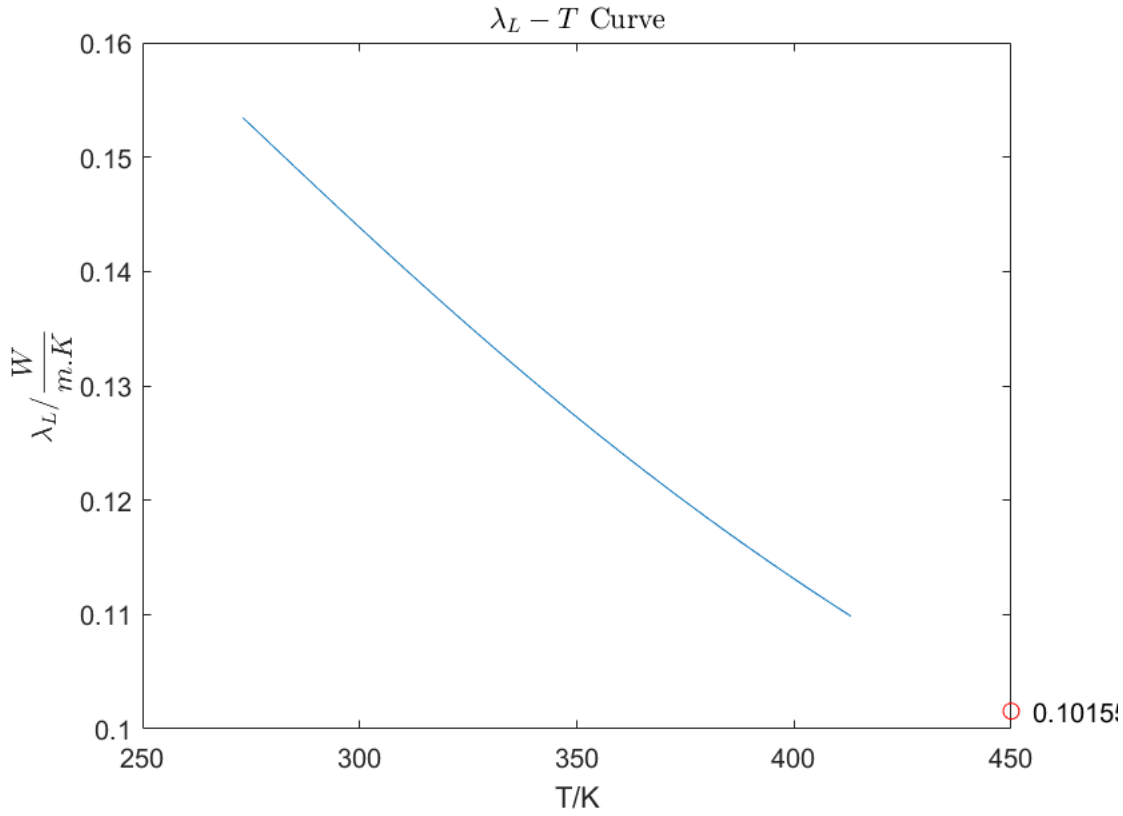
- VaporViscosity, 气体粘度, Pa.s
- $$\mu_V = \frac{A * T^B}{\left(1 + \frac{C}{T} + \frac{D}{T^2}\right)}$$

```
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')
```



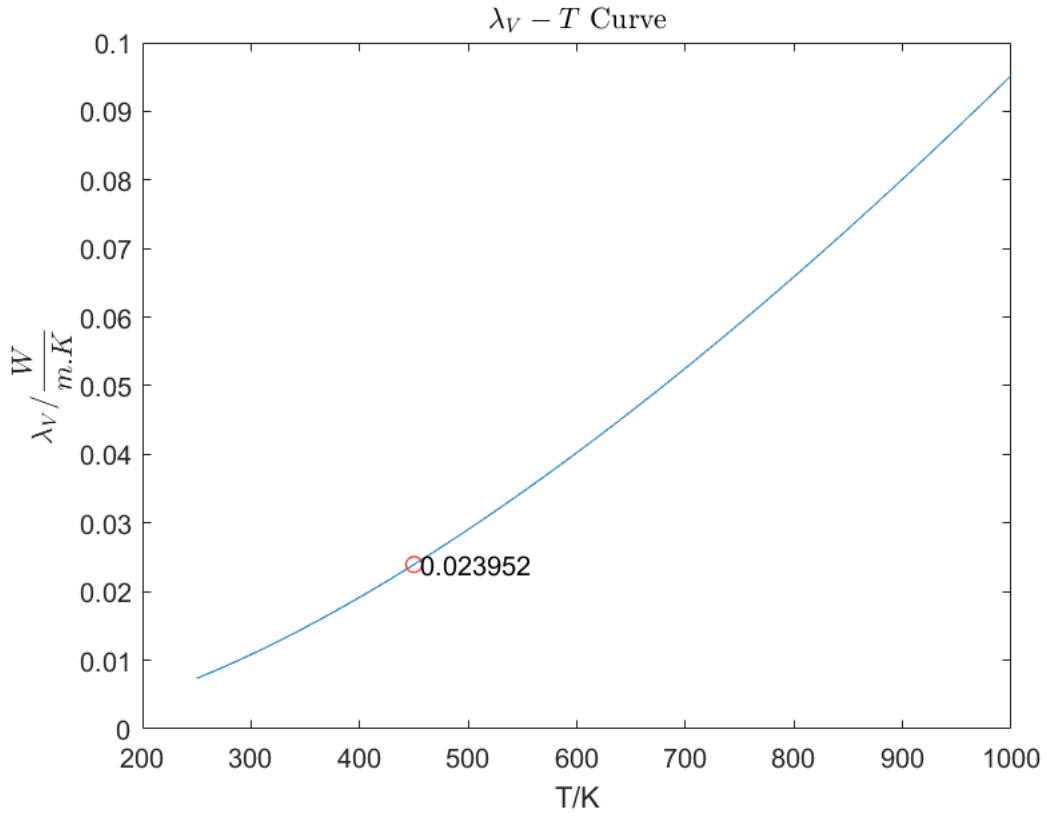
- LiquidThermalConductivity, 液体导热系数, W/m/K
- $\lambda_L = A + e^{\left(\frac{B}{T}+C+D*T+E*T^2\right)}$

```
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')
```



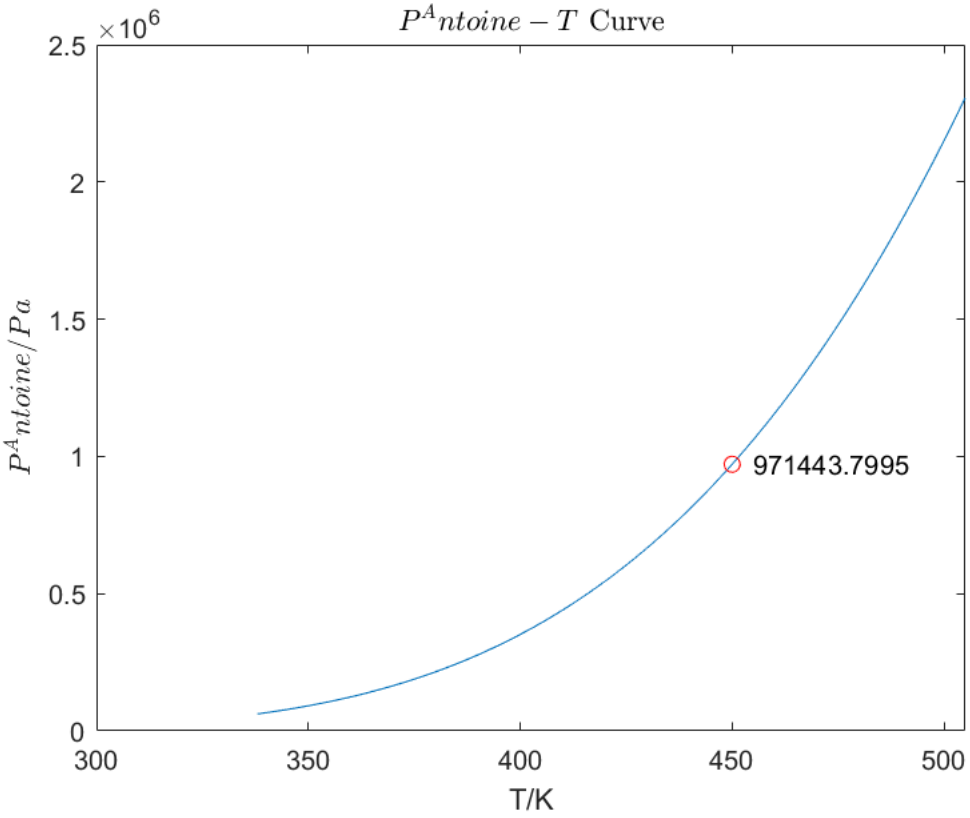
- VaporThermalConductivity, 气体导热系数, W/m/K
- $\lambda_V = \frac{A * T^B}{\left(1 + \frac{C}{T} + \frac{D}{T^2}\right)}$

```
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')
```



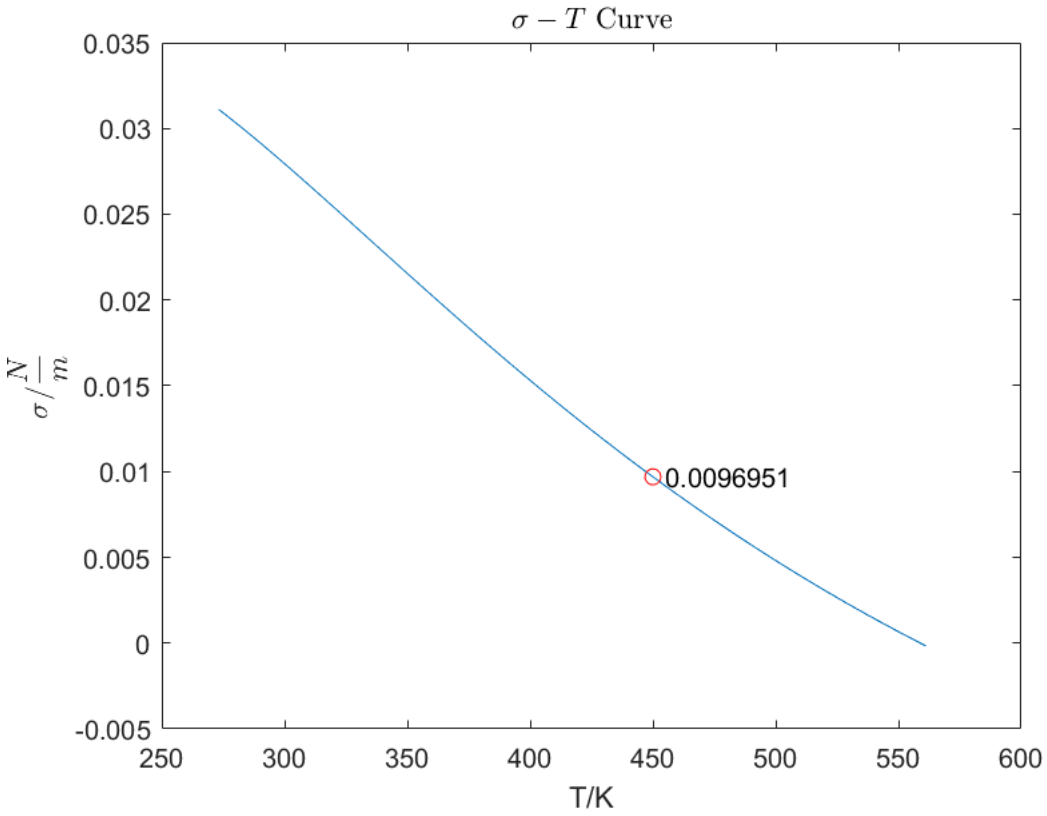
- AntoineVaporPressure, 安托因蒸汽压, Pa
- $P^{\text{Antoine}} = e^{\left(A - \frac{B}{(C+T)}\right)}$

```
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')
```



纯物质,丙烷为例,计算体积

```
% CAS = '74-98-6';
% CAS = '75-28-5';
% Propane = Component(CAS);
% P = 997420;
% P = 2190000;
% % P = 2250000
% T = 300;
% T = 400;
% z = 1;
% q = 1;
% [Vl,Hl] = EOS(P,T,z,q,Propane)
% q = 0;
% [Vv,Hv] = EOS(P,T,z,q,Propane)
% Hv-Hl
%
% P = 4247700;
% T = 369.85;
% q = 0;
% [Zcritical,Hcritical] = EOS(P,T,z,q,Propane);
% Vcritical = Zcritical*8.314*T/P;
```

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
% P = 15200000;
% T = 310.8;
% CH4 = Component('74-82-8');
% N2 = Component('7727-37-9');
% C2H6 = Component('74-84-0');
% z = [0.82,0.10,0.08];
% q = 0;
% [Zv,Hv1] = EOS(P,T,z,q,[CH4,N2,C2H6]);

CO2 = Component('124-38-9');
NC4 = Component('106-97-8');
P = 1.061*10^6;
T = 273.15;
z = [0.2,0.8];
q = 1;
EOS(P,T,z,q,[CO2,NC4]);
```

```
ans = -8.9749
ans = -7.4159
phi = 2×1
    1.4275
   -2.3056
```

```
z = [0.8962,0.1038];
q = 0;
EOS(P,T,z,q,[CO2,NC4]);
```

```
ans = -0.2874
ans = -0.1942
phi = 2×1
   -0.0751
   -0.2506
```

```
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));
% Sform, 绝对熵, J/kmol/K
Property.Sform = str2double(PropertyParameter.AbsEntropy(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 [V,phi,H] = EOS(P,T,z,q,Component)
    % Constant;
    % 理想气体常数J/koml/K
    R = 8.314 * 1000;
    % 基准温度Tref = 298.15,K
    % 基准压力Pref = 101325,Pa
    Tref = 298.15;
    Pref = 101325;

    c = length(z);
    z = z./sum(z);
    Pc = ones(c,1);
    Tc = ones(c,1);
    omega = ones(c,1);
    Mw = ones(c,1);
    Hideal_i = ones(c,1);
    S_temp_i = ones(c,1);
    Sideal_i = 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;
        Hideal_i(i) = integral(Component(i).IdealGasHeatCapacityCp_func, Tref, T);
        S_temp_i(i) = integral(@(T) Component(i).IdealGasHeatCapacityCp_func(T)/T, Tref, T, 'Ar
        Sideal_i(i) = Component(i).Sform;
```

```
end

% PR 方程系数
Omega_a = 0.45724;
Omega_b = 0.0778;
m = [0.37464, 1.54226, -0.2699];

fw_i = m(1) + m(2).*omega + m(3).*omega.^2;
alpha = (1+ fw_i.*(1-(T./Tc).^0.5) ).^2;
ac_i = Omega_a.*R.^2.*Tc.^2./Pc;
a_i = ac_i.* alpha;
b_i = Omega_b*R.*Tc./Pc;

% k,二元交互参数, c*c矩阵
kij = 0;

% 混合规则的选择
a_ij = (a_i*a_i').^0.5.*(1-kij);
b_ij = (b_i+b_i)/2;

a = z*a_ij*z';
b = z*b_ij;

% PR 方程delta,varepsilon,eta与a,b的关系式
delta = 2*b;
DELTA = delta*P/R/T;

varepsilon = -b^2;
VAREPSILON = varepsilon*(P/R/T)^2;

eta = b;
ETA = eta*P/R/T;

A = a*P/(R*T)^2;
B = b*P/R/T;

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 == 1, 液相
% q == 0, 气相
if q == 1
    Z = min(Z);
elseif q == 0
    Z = max(Z);
end

% 混合物的体积
V = Z*R*T/P;

% PR 方程的dadT
dadT = -z *( fw_i.*sqrt(a_i.*ac_i./T./Tc) );
```

```
    % 计算混合物的焓

    % 混合理想气体在研究态工况下的焓
    Hideal = z*Hideal_i;
    % 偏离焓的计算
    Temp1 = T*dadT - a;
    Temp2 = R*T*(delta^2-4*varepsilon)^0.5;
    Temp3 = 2*V+delta+(delta^2-4*varepsilon)^0.5;
    Temp4 = 2*V+delta-(delta^2-4*varepsilon)^0.5;
    Temp5 = log(Temp3/Temp4);
    HR = R*T*( Temp1 / Temp2*Temp5 +Z-1 );
    % 混合物的焓 = 理想气体的焓+偏离焓
    H = Hideal + HR;

    % 熵的计算目前还存在问题
    % 计算混合物的熵

    % 混合理想气体在研究态工况下的熵
    Sideal = z*(Sideal_i - R*log(P/Pref)-R*log(z') + S_temp_i);
    % 偏离熵的计算
    Temp1 =  R*(delta^2-4*varepsilon)^0.5;
    Temp2 = log(Temp3/Temp4);
    Temp5 = log(P*(V-b)/R/T);
    SR = R*(Temp5 + dadT/Temp1 * Temp2);
    S = Sideal + SR;

    % 计算混合物中组分i的系数系数
    Temp1 = b_i./b.*(Z-1)-log(Z-B);
    Temp2 = A./2^1.5/B.*(2*a_ij*z'./a - b_i./b);
    Temp3 = log( (Z+(1+sqrt(2))*B)./(Z+(1-sqrt(2))*B) );
    phi = exp(Temp1-Temp2.*Temp3);

end
```