

# Thermodynamic and transport properties of gases

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Specific heat at constant pressure:

$$\frac{c_p}{R} = \frac{\hat{c}_p}{\hat{R}} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

where  $\hat{R} = 8.31447 \text{ kJ/kmolK}$ ; the value of the coefficients are given below for different gases; temperatures in K.

Absolute enthalpy (formation enthalpy is included) at  $p = 1 \text{ atm}$ :

$$\frac{h^o(T)}{RT} = \frac{\hat{h}^o(T)}{\hat{R}T} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T}$$

Temperatures in K.

Absolute entropy at  $p = 1 \text{ atm}$ :

$$\frac{s^o(T)}{R} = \frac{\hat{s}^o(T)}{\hat{R}} = a_1 \ln(T) + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7$$

Temperatures in K.

Dynamic viscosity and thermal conductivity:

$$\mu \left( \frac{\text{kg}}{\text{ms}} \right) = e^{b_0 + b_1 \ln T + b_2 (\ln T)^2 + a_3 (\ln T)^3}; \quad \lambda \left( \frac{\text{W}}{\text{mK}} \right) = e^{c_0 + c_1 \ln T + c_2 (\ln T)^2 + c_3 (\ln T)^3}$$

Temperatures in K.

Coefficients for different gases of the polynomial expressions given below for. The coefficients corresponding to the thermodynamic properties ( $c_p$ ,  $h^o$  and  $s^o$ ) have been obtained from JANAF<sup>1</sup>. Transport properties ( $\mu$  and  $\lambda$ ) from CHEMKIN<sup>2</sup>.

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## AR Argon

JANAF-CHEMKIN

MW 0.3994800186e+02 (molecular mass in kg/kmol)

2

200.0 1000.0 (temperature range from 200 to 1000 K)

				$b_0, b_1, b_2, b_3$	$c_0, c_1, c_2, c_3$	$a_0, a_1, a_2, \dots$
RO	GASIDEAL					
MU	EPOLI3	-0.2133949627e+02	0.3467381630e+01	-0.3746257298e+00	0.1658331947e-01	
LAMBDA	EPOLI3	-0.1467956128e+02	0.3467381630e+01	-0.3746257298e+00	0.1658331947e-01	
CP	JANAF_CP	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00
H	JANAF_H	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00
S	JANAF_S	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00

1000.0 5000.0 (temperature range from 1000 to 5000 K)

RO	GASIDEAL					
MU	EPOLI3	-0.2133949627e+02	0.3467381630e+01	-0.3746257298e+00	0.1658331947e-01	
LAMBDA	EPOLI3	-0.1467956128e+02	0.3467381630e+01	-0.3746257298e+00	0.1658331947e-01	
CP	JANAF_CP	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00
H	JANAF_H	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00
S	JANAF_S	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00

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## C Carbon

JANAF-CHEMKIN

MW 0.1201115036e+02

2

200.0 1000.0

RO	GASIDEAL				
MU	EPOLI3	-0.1733304620e+02	0.1706343689e+01	-0.1443632622e+00	0.6539115412e-02
LAMBDA	EPOLI3	-0.9471367964e+01	0.1706343689e+01	-0.1443632622e+00	0.6539115412e-02
CP	JANAF_CP	0.2554239550e+01	-0.3215377240e-03	0.7337922450e-06	-0.7322348890e-09

1 See website: <http://www.sandia.gov/HiTempThermo/chemkin.html>. Note, similar correlations (but not the same) can be seen on the NIST website: <http://webbook.nist.gov/chemistry/>

2 See the same website: <http://www.sandia.gov/HiTempThermo/chemkin.html>.

H	JANAF_H	0.2554239550e+01	-0.3215377240e-03	0.7337922450e-06	-0.7322348890e-09	0.2665214460e-12	0.8544388320e+05
S	JANAF_S	0.2554239550e+01	-0.3215377240e-03	0.7337922450e-06	-0.7322348890e-09	0.2665214460e-12	0.4531308480e+01

1000.0 5000.0

RO	GASIDEAL						
MU	EPOLI3	-0.1733304620e+02	0.1706343689e+01	-0.1443632622e+00	0.6539115412e-02		
LAMBDA	EPOLI3	-0.9471367964e+01	0.1706343689e+01	-0.1443632622e+00	0.6539115412e-02		
CP	JANAF_CP	0.2492668880e+01	0.4798892840e-04	-0.7243350200e-07	0.3742910290e-10	-0.4872778930e-14	
H	JANAF_H	0.2492668880e+01	0.4798892840e-04	-0.7243350200e-07	0.3742910290e-10	-0.4872778930e-14	0.8545129530e+05
S	JANAF_S	0.2492668880e+01	0.4798892840e-04	-0.7243350200e-07	0.3742910290e-10	-0.4872778930e-14	0.4801503730e+01

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#### CH4 Methane

JANAF-CHEMKIN

MW 0.1604303026e+02

2

200.0 1000.0

RO	GASIDEAL						
MU	EPOLI3	-0.2230715913e+02	0.3569542093e+01	-0.3874920393e+00	0.1712461411e-01		
LAMBDA	EPOLI3	0.1793259165e+01	-0.4960294457e+01	0.1032808843e+01	-0.5633567903e-01		
CP	JANAF_CP	0.5149876130e+01	-0.1367097880e-01	0.4918005990e-04	-0.4847430260e-07	0.1666939560e-10	
H	JANAF_H	0.5149876130e+01	-0.1367097880e-01	0.4918005990e-04	-0.4847430260e-07	0.1666939560e-10	-0.1024664760e+05
S	JANAF_S	0.5149876130e+01	-0.1367097880e-01	0.4918005990e-04	-0.4847430260e-07	0.1666939560e-10	-0.4641303760e+01

1000.0 5000.0

RO	GASIDEAL						
MU	EPOLI3	-0.2230715913e+02	0.3569542093e+01	-0.3874920393e+00	0.1712461411e-01		
LAMBDA	EPOLI3	0.1793259165e+01	-0.4960294457e+01	0.1032808843e+01	-0.5633567903e-01		
CP	JANAF_CP	0.7485149500e-01	0.1339094670e-01	-0.5732858090e-05	0.1222925350e-08	-0.1018152300e-12	
H	JANAF_H	0.7485149500e-01	0.1339094670e-01	-0.5732858090e-05	0.1222925350e-08	-0.1018152300e-12	-0.9468344590e+04
S	JANAF_S	0.7485149500e-01	0.1339094670e-01	-0.5732858090e-05	0.1222925350e-08	-0.1018152300e-12	0.1843731800e+02

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#### CO Carbon monoxide

JANAF-CHEMKIN

MW 0.2801055050e+02

2

200.0 1000.0

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RO  GASIDEAL
MU  EPOLI3 -0.1891819775e+02  0.2400975158e+01 -0.2357717790e+00  0.1054820948e-01
LAMBDA EPOLI3  0.3641755785e+00 -0.3154801253e+01  0.6020483455e+00 -0.3032714733e-01
CP  JANAF_CP 0.3579533470e+01 -0.6103536800e-03  0.1016814330e-05  0.9070058840e-09 -0.9044244990e-12
H   JANAF_H  0.3579533470e+01 -0.6103536800e-03  0.1016814330e-05  0.9070058840e-09 -0.9044244990e-12 -0.1434408600e+05
S   JANAF_S  0.3579533470e+01 -0.6103536800e-03  0.1016814330e-05  0.9070058840e-09 -0.9044244990e-12  0.3508409280e+01

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1000.0 5000.0

```

RO  GASIDEAL
MU  EPOLI3 -0.1891819775e+02  0.2400975158e+01 -0.2357717790e+00  0.1054820948e-01
LAMBDA EPOLI3  0.3641755785e+00 -0.3154801253e+01  0.6020483455e+00 -0.3032714733e-01
CP  JANAF_CP 0.2715185610e+01  0.2062527430e-02 -0.9988257710e-06  0.2300530080e-09 -0.2036477160e-13
H   JANAF_H  0.2715185610e+01  0.2062527430e-02 -0.9988257710e-06  0.2300530080e-09 -0.2036477160e-13 -0.1415187240e+05
S   JANAF_S  0.2715185610e+01  0.2062527430e-02 -0.9988257710e-06  0.2300530080e-09 -0.2036477160e-13  0.7818687720e+01

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## CO2 Carbon dioxide

JANAF-CHEMKIN

MW 0.4400995064e+02

2

200.0 1000.0

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RO  GASIDEAL
MU  EPOLI3 -0.2627315808e+02  0.5130426196e+01 -0.5724284704e+00  0.2440888722e-01
LAMBDA EPOLI3 -0.2286363338e+02  0.5875667874e+01 -0.5677982250e+00  0.2031670239e-01
CP  JANAF_CP 0.2356773520e+01  0.8984596770e-02 -0.7123562690e-05  0.2459190220e-08 -0.1436995480e-12
H   JANAF_H  0.2356773520e+01  0.8984596770e-02 -0.7123562690e-05  0.2459190220e-08 -0.1436995480e-12 -0.4837196970e+05
S   JANAF_S  0.2356773520e+01  0.8984596770e-02 -0.7123562690e-05  0.2459190220e-08 -0.1436995480e-12  0.9901052220e+01

```

1000.0 5000.0

```

RO  GASIDEAL
MU  EPOLI3 -0.2627315808e+02  0.5130426196e+01 -0.5724284704e+00  0.2440888722e-01
LAMBDA EPOLI3 -0.2286363338e+02  0.5875667874e+01 -0.5677982250e+00  0.2031670239e-01
CP  JANAF_CP 0.3857460290e+01  0.4414370260e-02 -0.2214814040e-05  0.5234901880e-09 -0.4720841640e-13
H   JANAF_H  0.3857460290e+01  0.4414370260e-02 -0.2214814040e-05  0.5234901880e-09 -0.4720841640e-13 -0.4875916600e+05
S   JANAF_S  0.3857460290e+01  0.4414370260e-02 -0.2214814040e-05  0.5234901880e-09 -0.4720841640e-13  0.2271638060e+01

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## H Hydrogen atom

JANAF-CHEMKIN

MW 0.1007969975e+01

2

200.0 1000.0

RO GASIDEAL

MU EPOLI3 -0.2270792854e+02 0.3652691486e+01 -0.3980303021e+00 0.1757072886e-01

LAMBDA EPOLI3 -0.1236835327e+02 0.3652691486e+01 -0.3980303021e+00 0.1757072886e-01

CP JANAF\_CP 0.2500000000e+01 0.7053328190e-12 -0.1995919640e-14 0.2300816320e-17 -0.9277323320e-21

H JANAF\_H 0.2500000000e+01 0.7053328190e-12 -0.1995919640e-14 0.2300816320e-17 -0.9277323320e-21 0.2547365990e+05

S JANAF\_S 0.2500000000e+01 0.7053328190e-12 -0.1995919640e-14 0.2300816320e-17 -0.9277323320e-21 -0.4466828530e+00

1000.0 5000.0

RO GASIDEAL

MU EPOLI3 -0.2270792854e+02 0.3652691486e+01 -0.3980303021e+00 0.1757072886e-01

LAMBDA EPOLI3 -0.1236835327e+02 0.3652691486e+01 -0.3980303021e+00 0.1757072886e-01

CP JANAF\_CP 0.2500000010e+01 -0.2308429730e-10 0.1615619480e-13 -0.4735152350e-17 0.4981973570e-21

H JANAF\_H 0.2500000010e+01 -0.2308429730e-10 0.1615619480e-13 -0.4735152350e-17 0.4981973570e-21 0.2547365990e+05

S JANAF\_S 0.2500000010e+01 -0.2308429730e-10 0.1615619480e-13 -0.4735152350e-17 0.4981973570e-21 -0.4466829140e+00

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## H2 Hydrogen

JANAF-CHEMKIN

MW 0.2015939951e+01

2

200.0 1000.0

RO GASIDEAL

MU EPOLI3 -0.1614293964e+02 0.1003491326e+01 -0.5016044555e-01 0.2330995224e-02

LAMBDA EPOLI3 -0.2277096638e+01 -0.4674267764e+00 0.1156734789e+00 -0.2596025563e-02

CP JANAF\_CP 0.2344331120e+01 0.7980520750e-02 -0.1947815100e-04 0.2015720940e-07 -0.7376117610e-11

H JANAF\_H 0.2344331120e+01 0.7980520750e-02 -0.1947815100e-04 0.2015720940e-07 -0.7376117610e-11 -0.9179351730e+03

S JANAF\_S 0.2344331120e+01 0.7980520750e-02 -0.1947815100e-04 0.2015720940e-07 -0.7376117610e-11 0.6830102380e+00

1000.0 5000.0

RO GASIDEAL

MU EPOLI3 -0.1614293964e+02 0.1003491326e+01 -0.5016044555e-01 0.2330995224e-02

LAMBDA EPOLI3 -0.2277096638e+01 -0.4674267764e+00 0.1156734789e+00 -0.2596025563e-02

CP JANAF\_CP 0.3337279200e+01 -0.4940247310e-04 0.4994567780e-06 -0.1795663940e-09 0.2002553760e-13

H JANAF\_H 0.3337279200e+01 -0.4940247310e-04 0.4994567780e-06 -0.1795663940e-09 0.2002553760e-13 -0.9501589220e+03

S JANAF\_S 0.3337279200e+01 -0.4940247310e-04 0.4994567780e-06 -0.1795663940e-09 0.2002553760e-13 -0.3205023310e+01

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**H2O Water**

JANAF-CHEMKIN

MW 0.1801534009e+02

2

200.0 1000.0

RO GASIDEAL

MU EPOLI3 -0.1286013492e+02 -0.1377850379e+01 0.4213981638e+00 -0.2414423056e-01

LAMBDA EPOLI3 0.1185254026e+02 -0.8965822807e+01 0.1528828068e+01 -0.7590175979e-01

CP JANAF\_CP 0.4198640560e+01 -0.2036434100e-02 0.6520402110e-05 -0.5487970620e-08 0.1771978170e-11

H JANAF\_H 0.4198640560e+01 -0.2036434100e-02 0.6520402110e-05 -0.5487970620e-08 0.1771978170e-11 -0.3029372670e+05

S JANAF\_S 0.4198640560e+01 -0.2036434100e-02 0.6520402110e-05 -0.5487970620e-08 0.1771978170e-11 -0.8490322080e+00

1000.0 5000.0

RO GASIDEAL

MU EPOLI3 -0.1286013492e+02 -0.1377850379e+01 0.4213981638e+00 -0.2414423056e-01

LAMBDA EPOLI3 0.1185254026e+02 -0.8965822807e+01 0.1528828068e+01 -0.7590175979e-01

CP JANAF\_CP 0.3033992490e+01 0.2176918040e-02 -0.1640725180e-06 -0.9704198700e-10 0.1682009920e-13

H JANAF\_H 0.3033992490e+01 0.2176918040e-02 -0.1640725180e-06 -0.9704198700e-10 0.1682009920e-13 -0.3000429710e+05

S JANAF\_S 0.3033992490e+01 0.2176918040e-02 -0.1640725180e-06 -0.9704198700e-10 0.1682009920e-13 0.4966770100e+01

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**H2O2 Peroxide**

JANAF-CHEMKIN

MW 0.3401474023e+02

2

200.0 1000.0

RO GASIDEAL

MU EPOLI3 -0.1943012788e+02 0.2678088349e+01 -0.2721592408e+00 0.1214173233e-01

LAMBDA EPOLI3 -0.1063014819e+02 0.1315528335e+01 0.1916184484e-01 -0.4416817199e-02

CP JANAF\_CP 0.4276112690e+01 -0.5428224170e-03 0.1673357010e-04 -0.2157708130e-07 0.8624543630e-11

H JANAF\_H 0.4276112690e+01 -0.5428224170e-03 0.1673357010e-04 -0.2157708130e-07 0.8624543630e-11 -0.1770258210e+05

S JANAF\_S 0.4276112690e+01 -0.5428224170e-03 0.1673357010e-04 -0.2157708130e-07 0.8624543630e-11 0.3435050740e+01

1000.0 5000.0

RO GASIDEAL

MU EPOLI3 -0.1943012788e+02 0.2678088349e+01 -0.2721592408e+00 0.1214173233e-01

```
LAMBDA EPOLI3 -0.1063014819e+02 0.1315528335e+01 0.1916184484e-01 -0.4416817199e-02
CP JANAF_CP 0.4165002850e+01 0.4908316940e-02 -0.1901392250e-05 0.3711859860e-09 -0.2879083050e-13
H JANAF_H 0.4165002850e+01 0.4908316940e-02 -0.1901392250e-05 0.3711859860e-09 -0.2879083050e-13 -0.1786178770e+05
S JANAF_S 0.4165002850e+01 0.4908316940e-02 -0.1901392250e-05 0.3711859860e-09 -0.2879083050e-13 0.2916156620e+01
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## HO2 Hydroperoxyl

JANAF-CHEMKIN

MW 0.3300677025e+02

2

200.0 1000.0

```
RO GASIDEAL
MU EPOLI3 -0.1944516852e+02 0.2678088349e+01 -0.2721592408e+00 0.1214173233e-01
LAMBDA EPOLI3 -0.1264302144e+02 0.2340066563e+01 -0.1632055933e+00 0.5799980518e-02
CP JANAF_CP 0.4301798010e+01 -0.4749120510e-02 0.2115828910e-04 -0.2427638940e-07 0.9292251240e-11
H JANAF_H 0.4301798010e+01 -0.4749120510e-02 0.2115828910e-04 -0.2427638940e-07 0.9292251240e-11 0.2948080400e+03
S JANAF_S 0.4301798010e+01 -0.4749120510e-02 0.2115828910e-04 -0.2427638940e-07 0.9292251240e-11 0.3716662450e+01
```

1000.0 5000.0

```
RO GASIDEAL
MU EPOLI3 -0.1944516852e+02 0.2678088349e+01 -0.2721592408e+00 0.1214173233e-01
LAMBDA EPOLI3 -0.1264302144e+02 0.2340066563e+01 -0.1632055933e+00 0.5799980518e-02
CP JANAF_CP 0.4017210900e+01 0.2239820130e-02 -0.6336581500e-06 0.1142463700e-09 -0.1079085350e-13
H JANAF_H 0.4017210900e+01 0.2239820130e-02 -0.6336581500e-06 0.1142463700e-09 -0.1079085350e-13 0.1118567130e+03
S JANAF_S 0.4017210900e+01 0.2239820130e-02 -0.6336581500e-06 0.1142463700e-09 -0.1079085350e-13 0.3785102150e+01
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## N Nitrogen atom

JANAF-CHEMKIN

MW 0.1400669956e+02

2

200.0 1000.0

```
RO GASIDEAL
MU EPOLI3 -0.1725619603e+02 0.1706343689e+01 -0.1443632622e+00 0.6539115412e-02
LAMBDA EPOLI3 -0.9548218134e+01 0.1706343689e+01 -0.1443632622e+00 0.6539115412e-02
CP JANAF_CP 0.2500000000e+01 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00
H JANAF_H 0.2500000000e+01 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.5610463700e+05
S JANAF_S 0.2500000000e+01 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.0000000000e+00 0.4193908700e+01
```

1000.0 5000.0

```

RO  GASIDEAL
MU  EPOLI3  -0.1725619603e+02  0.1706343689e+01  -0.1443632622e+00  0.6539115412e-02
LAMBDA EPOLI3  -0.9548218134e+01  0.1706343689e+01  -0.1443632622e+00  0.6539115412e-02
CP  JANAF_CP  0.2415942900e+01  0.1748906500e-03  -0.1190236900e-06  0.3022624500e-10  -0.2036098200e-14
H   JANAF_H   0.2415942900e+01  0.1748906500e-03  -0.1190236900e-06  0.3022624500e-10  -0.2036098200e-14  0.5613377300e+05
S   JANAF_S   0.2415942900e+01  0.1748906500e-03  -0.1190236900e-06  0.3022624500e-10  -0.2036098200e-14  0.4649609600e+01

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## N2 Nitrogen

JANAF-CHEMKIN

MW 0.2801339912e+02

2

200.0 1000.0

```

RO  GASIDEAL
MU  EPOLI3  -0.1886822179e+02  0.2388167036e+01  -0.2341208183e+00  0.1047727173e-01
LAMBDA EPOLI3  0.1417117599e+01  -0.3528374680e+01  0.6455829015e+00  -0.3194413600e-01
CP  JANAF_CP  0.3298677000e+01  0.1408240400e-02  -0.3963222000e-05  0.5641515000e-08  -0.2444854000e-11
H   JANAF_H   0.3298677000e+01  0.1408240400e-02  -0.3963222000e-05  0.5641515000e-08  -0.2444854000e-11  -0.1020899900e+04
S   JANAF_S   0.3298677000e+01  0.1408240400e-02  -0.3963222000e-05  0.5641515000e-08  -0.2444854000e-11  0.3950372000e+01

```

1000.0 5000.0

```

RO  GASIDEAL
MU  EPOLI3  -0.1886822179e+02  0.2388167036e+01  -0.2341208183e+00  0.1047727173e-01
LAMBDA EPOLI3  0.1417117599e+01  -0.3528374680e+01  0.6455829015e+00  -0.3194413600e-01
CP  JANAF_CP  0.2926640000e+01  0.1487976800e-02  -0.5684760000e-06  0.1009703800e-09  -0.6753351000e-14
H   JANAF_H   0.2926640000e+01  0.1487976800e-02  -0.5684760000e-06  0.1009703800e-09  -0.6753351000e-14  -0.9227977000e+03
S   JANAF_S   0.2926640000e+01  0.1487976800e-02  -0.5684760000e-06  0.1009703800e-09  -0.6753351000e-14  0.5980528000e+01

```

#-----

## N2O ---

JANAF-CHEMKIN

MW 0.4401279926e+02

2

200.0 1000.0

```

RO  GASIDEAL
MU  EPOLI3  -0.2607150910e+02  0.5067455296e+01  -0.5674645603e+00  0.2432611681e-01
LAMBDA EPOLI3  -0.2297207455e+02  0.6034436002e+01  -0.6061276742e+00  0.2281390045e-01

```



CP	JANAF_CP	0.2257150200e+01	0.1130472800e-01	-0.1367131900e-04	0.9681980600e-08	-0.2930718200e-11	
H	JANAF_H	0.2257150200e+01	0.1130472800e-01	-0.1367131900e-04	0.9681980600e-08	-0.2930718200e-11	0.8741774400e+04
S	JANAF_S	0.2257150200e+01	0.1130472800e-01	-0.1367131900e-04	0.9681980600e-08	-0.2930718200e-11	0.1075799200e+02

1000.0 5000.0

RO	GASIDEAL						
MU	EPOLI3	-0.2607150910e+02	0.5067455296e+01	-0.5674645603e+00	0.2432611681e-01		
LAMBDA	EPOLI3	-0.2297207455e+02	0.6034436002e+01	-0.6061276742e+00	0.2281390045e-01		
CP	JANAF_CP	0.4823072900e+01	0.2627025100e-02	-0.9585087400e-06	0.1600071200e-09	-0.9775230300e-14	
H	JANAF_H	0.4823072900e+01	0.2627025100e-02	-0.9585087400e-06	0.1600071200e-09	-0.9775230300e-14	0.8073404800e+04
S	JANAF_S	0.4823072900e+01	0.2627025100e-02	-0.9585087400e-06	0.1600071200e-09	-0.9775230300e-14	-0.2201720700e+01

#-----

## NO Nitrogen monoxide

JANAF-CHEMKIN

MW 0.3000609970e+02

2

200.0 1000.0

RO	GASIDEAL						
MU	EPOLI3	-0.1883386291e+02	0.2388167036e+01	-0.2341208183e+00	0.1047727173e-01		
LAMBDA	EPOLI3	-0.1947028576e+01	-0.2131168801e+01	0.4544282044e+00	-0.2335117715e-01		
CP	JANAF_CP	0.4218476300e+01	-0.4638976000e-02	0.1104102200e-04	-0.9336135400e-08	0.2803577000e-11	
H	JANAF_H	0.4218476300e+01	-0.4638976000e-02	0.1104102200e-04	-0.9336135400e-08	0.2803577000e-11	0.9844623000e+04
S	JANAF_S	0.4218476300e+01	-0.4638976000e-02	0.1104102200e-04	-0.9336135400e-08	0.2803577000e-11	0.2280846400e+01

1000.0 5000.0

RO	GASIDEAL						
MU	EPOLI3	-0.1883386291e+02	0.2388167036e+01	-0.2341208183e+00	0.1047727173e-01		
LAMBDA	EPOLI3	-0.1947028576e+01	-0.2131168801e+01	0.4544282044e+00	-0.2335117715e-01		
CP	JANAF_CP	0.3260605600e+01	0.1191104300e-02	-0.4291704800e-06	0.6945766900e-10	-0.4033609900e-14	
H	JANAF_H	0.3260605600e+01	0.1191104300e-02	-0.4291704800e-06	0.6945766900e-10	-0.4033609900e-14	0.9920974600e+04
S	JANAF_S	0.3260605600e+01	0.1191104300e-02	-0.4291704800e-06	0.6945766900e-10	-0.4033609900e-14	0.6369302700e+01

#-----

## NO2 Nitrogen dioxide

JANAF-CHEMKIN

MW 0.4600549984e+02

2

200.0 1000.0

```
RO  GASIDEAL
MU  EPOLI3  -0.2468321217e+02  0.4668511699e+01  -0.5223152219e+00  0.2264144496e-01
LAMBDA EPOLI3  -0.2541446897e+02  0.7263546623e+01  -0.7968863012e+00  0.3249189251e-01
CP  JANAF_CP  0.3944031200e+01  -0.1585429000e-02  0.1665781200e-04  -0.2047542600e-07  0.7835056400e-11
H   JANAF_H   0.3944031200e+01  -0.1585429000e-02  0.1665781200e-04  -0.2047542600e-07  0.7835056400e-11  0.2896617900e+04
S   JANAF_S   0.3944031200e+01  -0.1585429000e-02  0.1665781200e-04  -0.2047542600e-07  0.7835056400e-11  0.6311991700e+01
```

1000.0 5000.0

```
RO  GASIDEAL
MU  EPOLI3  -0.2468321217e+02  0.4668511699e+01  -0.5223152219e+00  0.2264144496e-01
LAMBDA EPOLI3  -0.2541446897e+02  0.7263546623e+01  -0.7968863012e+00  0.3249189251e-01
CP  JANAF_CP  0.4884754200e+01  0.2172395600e-02  -0.8280690600e-06  0.1574751000e-09  -0.1051089500e-13
H   JANAF_H   0.4884754200e+01  0.2172395600e-02  -0.8280690600e-06  0.1574751000e-09  -0.1051089500e-13  0.2316498300e+04
S   JANAF_S   0.4884754200e+01  0.2172395600e-02  -0.8280690600e-06  0.1574751000e-09  -0.1051089500e-13  -0.1174169500e+00
```

#-----

## O Oxygen atom

JANAF-CHEMKIN

MW 0.1599940014e+02

2

200.0 1000.0

```
RO  GASIDEAL
MU  EPOLI3  -0.1740286218e+02  0.1929024678e+01  -0.1738657445e+00  0.7841476915e-02
LAMBDA EPOLI3  -0.9827899765e+01  0.1929024678e+01  -0.1738657445e+00  0.7841476915e-02
CP  JANAF_CP  0.3168267100e+01  -0.3279318840e-02  0.6643063960e-05  -0.6128066240e-08  0.2112659710e-11
H   JANAF_H   0.3168267100e+01  -0.3279318840e-02  0.6643063960e-05  -0.6128066240e-08  0.2112659710e-11  0.2912225920e+05
S   JANAF_S   0.3168267100e+01  -0.3279318840e-02  0.6643063960e-05  -0.6128066240e-08  0.2112659710e-11  0.2051933460e+01
```

1000.0 5000.0

```
RO  GASIDEAL
MU  EPOLI3  -0.1740286218e+02  0.1929024678e+01  -0.1738657445e+00  0.7841476915e-02
LAMBDA EPOLI3  -0.9827899765e+01  0.1929024678e+01  -0.1738657445e+00  0.7841476915e-02
CP  JANAF_CP  0.2569420780e+01  -0.8597411370e-04  0.4194845890e-07  -0.1001777990e-10  0.1228336910e-14
H   JANAF_H   0.2569420780e+01  -0.8597411370e-04  0.4194845890e-07  -0.1001777990e-10  0.1228336910e-14  0.2921757910e+05
S   JANAF_S   0.2569420780e+01  -0.8597411370e-04  0.4194845890e-07  -0.1001777990e-10  0.1228336910e-14  0.4784338640e+01
```

#-----

## O2 Oxygen

JANAF-CHEMKIN

MW 0.3199880028e+02

2

200.0 1000.0

RO GASIDEAL

MU EPOLI3 -0.1946067566e+02 0.2678088349e+01 -0.2721592408e+00 0.1214173233e-01

LAMBDA EPOLI3 -0.1344962361e+02 0.2890477542e+01 -0.2709591162e+00 0.1152570281e-01

CP JANAF\_CP 0.3782456360e+01 -0.2996734160e-02 0.9847302010e-05 -0.9681295090e-08 0.3243728370e-11

H JANAF\_H 0.3782456360e+01 -0.2996734160e-02 0.9847302010e-05 -0.9681295090e-08 0.3243728370e-11 -0.1063943560e+04

S JANAF\_S 0.3782456360e+01 -0.2996734160e-02 0.9847302010e-05 -0.9681295090e-08 0.3243728370e-11 0.3657675730e+01

1000.0 5000.0

RO GASIDEAL

MU EPOLI3 -0.1946067566e+02 0.2678088349e+01 -0.2721592408e+00 0.1214173233e-01

LAMBDA EPOLI3 -0.1344962361e+02 0.2890477542e+01 -0.2709591162e+00 0.1152570281e-01

CP JANAF\_CP 0.3282537840e+01 0.1483087540e-02 -0.7579666690e-06 0.2094705550e-09 -0.2167177940e-13

H JANAF\_H 0.3282537840e+01 0.1483087540e-02 -0.7579666690e-06 0.2094705550e-09 -0.2167177940e-13 -0.1088457720e+04

S JANAF\_S 0.3282537840e+01 0.1483087540e-02 -0.7579666690e-06 0.2094705550e-09 -0.2167177940e-13 0.5453231290e+01

#-----

**OH Hydroxil**

JANAF-CHEMKIN

MW 0.1700737011e+02

2

200.0 1000.0

RO GASIDEAL

MU EPOLI3 -0.1737231441e+02 0.1929024678e+01 -0.1738657445e+00 0.7841476915e-02

LAMBDA EPOLI3 0.2649305782e+01 -0.3244626711e+01 0.5336588173e+00 -0.2328116832e-01

CP JANAF\_CP 0.3992015430e+01 -0.2401317520e-02 0.4617938410e-05 -0.3881133330e-08 0.1364114700e-11

H JANAF\_H 0.3992015430e+01 -0.2401317520e-02 0.4617938410e-05 -0.3881133330e-08 0.1364114700e-11 0.3615080560e+04

S JANAF\_S 0.3992015430e+01 -0.2401317520e-02 0.4617938410e-05 -0.3881133330e-08 0.1364114700e-11 -0.1039254580e+00

1000.0 5000.0

RO GASIDEAL

MU EPOLI3 -0.1737231441e+02 0.1929024678e+01 -0.1738657445e+00 0.7841476915e-02

LAMBDA EPOLI3 0.2649305782e+01 -0.3244626711e+01 0.5336588173e+00 -0.2328116832e-01

CP JANAF\_CP 0.3092887670e+01 0.5484297160e-03 0.1265052280e-06 -0.8794615560e-10 0.1174123760e-13

H JANAF\_H 0.3092887670e+01 0.5484297160e-03 0.1265052280e-06 -0.8794615560e-10 0.1174123760e-13 0.3858657000e+04

```

S JANAF_S 0.3092887670e+01 0.5484297160e-03 0.1265052280e-06 -0.8794615560e-10 0.1174123760e-13 0.4476696100e+01
#-----
C2H2 Acetylene
JANAF-CHEMKIN
MW 0.2603824067e+02
2
200.0 1000.0

RO GASIDEAL
MU EPOLI3 -0.2563911990e+02 0.4790351552e+01 -0.5364560276e+00 0.2318560947e-01
LAMBDA EPOLI3 -0.1920397367e+02 0.4564166690e+01 -0.4040787948e+00 0.1405248078e-01
CP JANAF_CP 0.8086810940e+00 0.2336156290e-01 -0.3551718150e-04 0.2801524370e-07 -0.8500729740e-11
H JANAF_H 0.8086810940e+00 0.2336156290e-01 -0.3551718150e-04 0.2801524370e-07 -0.8500729740e-11 0.2642898070e+05
S JANAF_S 0.8086810940e+00 0.2336156290e-01 -0.3551718150e-04 0.2801524370e-07 -0.8500729740e-11 0.1393970510e+02

1000.0 5000.0

RO GASIDEAL
MU EPOLI3 -0.2563911990e+02 0.4790351552e+01 -0.5364560276e+00 0.2318560947e-01
LAMBDA EPOLI3 -0.1920397367e+02 0.4564166690e+01 -0.4040787948e+00 0.1405248078e-01
CP JANAF_CP 0.4147569640e+01 0.5961666640e-02 -0.2372948520e-05 0.4674121710e-09 -0.3612352130e-13
H JANAF_H 0.4147569640e+01 0.5961666640e-02 -0.2372948520e-05 0.4674121710e-09 -0.3612352130e-13 0.2593599920e+05
S JANAF_S 0.4147569640e+01 0.5961666640e-02 -0.2372948520e-05 0.4674121710e-09 -0.3612352130e-13 -0.1230281210e+01

```

#-----  
**C10H22 (n-decane) (gas) (ref. <http://webbook.nist.gov/chemistry/>)**

$$h_f^o = -249.7 \pm 1.1 \text{ kJ/mol}$$

$$s^o(298.15 \text{ K}) = 545.8 \pm 1.1 \text{ J/mol} \cdot \text{K}$$

Temperature (K)	200	273.15	298.15	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
c <sub>p,gas</sub> (J/mol*K)	179.08	217.9	233.1	234.18	297.98	356.43	405.85	446.43	479.9	508.36	531.79	551.87	569.44	585.76	598.31	610.86