

Thermodynamic and transport properties

Annex 1: Thermodynamic and transport properties (liquids and gases)

Annex 2: Thermodynamic and transport properties of gases (JANAF)

ANNEX 1. Thermodynamic and transport properties¹

Some gases and liquids fuels²:

- **Isobutene**, $C_4H_{10}(g)$, $\hat{h}_f^o = -126150 \text{ kJ/kmol}$, $\hat{c}_p(\text{kJ/kmolK}) = 35.6 + 0.2077 \cdot T (K)$, $LHV = 45.55 \text{ MJ/kg}$
- **n-Octane**, $C_8H_{18}(l)$, $\hat{h}_f^o = -249950 \text{ kJ/kmole}$, $\hat{c}_p = 254 \text{ kJ/kmolK}$, $LHV = 44.35 \text{ MJ/kg}$
- **n-Decane** (similar characteristics of kerosene), $C_{10}H_{22}(l)$, $\hat{h}_f^o = -294366 \text{ kJ/kmol}$, $\hat{c}_p = 296 \text{ kJ/kmolK}$, $LHV = 44.17 \text{ MJ/kg}$
- **Propane**, $C_3H_8(g)$, $\hat{c}_p(\text{kJ/kmolK}) = -4.04 + 30.48 \times 10^{-2}T - 15.72 \times 10^{-5}T^2 + 31.74 \times 10^{-9}T^3$, $T(K)$ range: $273 - 1500 \text{ K}$; $\hat{h}_f^o = -103850 \text{ kJ/kmol}$.

Table 1. Thermochemical properties of selected substances at 298 K and 1 atm

Substance	Formula	Molar mass, W (kg/kmol)	Enthalpy of formation, \hat{h}_f^o (kJ/kmol)	Gibbs function of formation, \hat{g}_f^o (kJ/kmol)	Absolute entropy, \hat{s}^o (kJ/kmol K)	Heating Values	
						Higher, HHV (kJ/kg)	Lower, LHV (kJ/kg)
Carbon	C(s)	12.01	0	0	5.74	32,770	32,770
Hydrogen	H ₂ (g)	2.016	0	0	130.57	141,780	119,950
Nitrogen	N ₂ (g)	28.01	0	0	191.50	—	—
Oxygen	O ₂ (g)	32.00	0	0	205.03	—	—
Carbon monoxide	CO(g)	28.01	-110,530	-137,150	197.54	—	—
Carbon dioxide	CO ₂ (g)	44.01	-393,520	-394,380	213.69	—	—
Water	H ₂ O(g)	18.02	-241,820	-228,590	188.72	—	—
Water	H ₂ O(l)	18.02	-285,830	-237,180	69.95	—	—
Hydrogen peroxide	H ₂ O ₂ (g)	34.02	-136,310	-105,600	232.63	—	—
Ammonia	NH ₃ (g)	17.03	-46,190	-16,590	192.33	—	—
Oxygen	O(g)	16.00	249,170	231,770	160.95	—	—
Hydrogen	H(g)	1.008	218,000	203,290	114.61	—	—
Nitrogen	N(g)	14.01	472,680	455,510	153.19	—	—
Hydroxyl	OH(g)	17.01	39,460	34,280	183.75	—	—
Methane	CH ₄ (g)	16.04	-74,850	-50,790	186.16	55,510	50,020
Acetylene	C ₂ H ₂ (g)	26.04	226,730	209,170	200.85	49,910	48,220
Ethylene	C ₂ H ₄ (g)	28.05	52,280	68,120	219.83	50,300	47,160
Ethane	C ₂ H ₆ (g)	30.07	-84,680	-32,890	229.49	51,870	47,480
Propylene	C ₃ H ₆ (g)	42.08	20,410	62,720	266.94	48,920	45,780
Propane	C ₃ H ₈ (g)	44.09	-103,850	-23,490	269.91	50,350	46,360
Pentane	C ₅ H ₁₂ (g)	72.15	-146,440	-8,200	348.40	49,010	45,350
Octane	C ₈ H ₁₈ (g)	114.22	-208,450	17,320	463.67	48,260	44,790
Octane	C ₈ H ₁₈ (l)	114.22	-249,910	6,610	360.79	47,900	44,430
Benzene	C ₆ H ₆ (g)	78.11	82,930	129,660	269.20	42,270	40,580
Methyl alcohol	CH ₃ OH(g)	32.04	-200,890	-162,140	239.70	23,850	21,110
Methyl alcohol	CH ₃ OH(l)	32.04	-238,810	-166,290	126.80	22,670	19,920
Ethyl alcohol	C ₂ H ₅ OH(g)	46.07	-235,310	-168,570	282.59	30,590	27,720
Ethyl alcohol	C ₂ H ₅ OH(l)	46.07	-277,690	-174,890	160.70	29,670	26,800

Source: Based on JANAF Thermochemical Tables, NSRDS-NBS-37, 1971; *Selected Values of Chemical Thermodynamic Properties*, NBS Tech. Note 270-3, 1968; and *API Research Project 44*, Carnegie Press, 1953. Heating values calculated.

¹ Note: Tables A25 and A-21 from M.J.Moran and H.N.Shapiro, *Fundamentals of Engineering Thermodynamics*, John Wiley & Sons, Inc.

² R.D.Flack, *Fundamentals of jet propulsion with applications*, Cambridge Aerospace Series, 2005.

Table 2. Specific heat for selected ideal gases (T in K ; range: $300 < T < 1000 K$)

$$\hat{c}_p/\hat{R} = c_p/R = \alpha + \beta T + \gamma T^2 + \delta T^3 + \varepsilon T^4$$

Gas	α	$\beta \times 10^3$	$\gamma \times 10^6$	$\delta \times 10^9$	$\varepsilon \times 10^{12}$
CO	3.710	-1.619	3.692	-2.032	0.240
CO ₂	2.401	8.735	-6.607	2.002	0
H ₂	3.057	2.677	-5.810	5.521	-1.812
H ₂ O	4.070	-1.108	4.152	-2.964	0.807
O ₂	3.626	-1.878	7.055	-6.764	2.156
N ₂	3.675	-1.208	2.324	-0.632	-0.226
Air	3.653	-1.337	3.294	-1.913	0.2763
SO ₂	3.267	5.324	0.684	-5.281	2.559
CH ₄	3.826	-3.979	24.558	-22.733	6.963
C ₂ H ₂	1.410	19.057	-24.501	16.391	-4.135
C ₂ H ₄	1.426	11.383	7.989	-16.254	6.749
Monatomic gases ^a	2.5	0	0	0	0

^aFor monatomic gases, such as He, Ne, and Ar, \bar{c}_p is constant over a wide temperature range and is very nearly equal to $5/2 \bar{R}$.

Source: Adapted from K. Wark, *Thermodynamics*, 4th ed., McGraw-Hill, New York, 1983, as based on NASA SP-273, U.S. Government Printing Office, Washington, DC, 1971.¹

Table 3. Flammability limits and ignition temperatures of common fuels in fuel/air mixtures

Substance	Molecular Formula	Lower Flammability Limit, %	Upper Flammability Limit, %	Ignition Temperature, °C	References
Carbon	C	—	—	660	Hartman (1958)
Carbon monoxide	CO	12.5	74	609	Scott et al. (1948)
Hydrogen	H ₂	4.0	75.0	520	Zabetakis (1956)
Methane	CH ₄	5.0	15.0	705	<i>Gas Engineers Handbook</i>
Ethane	C ₂ H ₆	3.0	12.5	520 to 630	Trinks (1947)
Propane	C ₃ H ₈	2.1	10.1	466	NFPA (1962)
<i>n</i> -Butane	C ₄ H ₁₀	1.86	8.41	405	NFPA (1962)
Ethylene	C ₂ H ₄	2.75	28.6	490	Scott et al. (1948)
Propylene	C ₃ H ₆	2.00	11.1	450	Scott et al. (1948)
Acetylene	C ₂ H ₂	2.50	81	406 to 440	Trinks (1947)
Sulfur	S	—	—	190	Hartman (1958)
Hydrogen sulfide	H ₂ S	4.3	45.50	292	Scott et al. (1948)

Flammability limits adapted from Coward and Jones (1952). All values corrected to 16°C, 104 kPa, dry. (% by volume of air)

ASHRAE Fundamentals

Table 4. Equilibrium constant K_p

Temp. K	$\log_{10} K$								Temp. °R
	$\text{H}_2 \rightleftharpoons 2\text{H}$	$\text{O}_2 \rightleftharpoons 2\text{O}$	$\text{N}_2 \rightleftharpoons 2\text{N}$	$\frac{1}{2}\text{O}_2 + \frac{1}{2}\text{N}_2 \rightleftharpoons \text{NO}$	$\text{H}_2\text{O} \rightleftharpoons \text{H}_2 + \frac{1}{2}\text{O}_2$	$\text{H}_2\text{O} \rightleftharpoons \text{OH} + \frac{1}{2}\text{H}_2$	$\text{CO}_2 \rightleftharpoons \text{CO} + \frac{1}{2}\text{O}_2$	$\text{CO}_2 + \text{H}_2 \rightleftharpoons \text{CO} + \text{H}_2\text{O}$	
298	-71.224	-81.208	-159.600	-15.171	-40.048	-46.054	-45.066	-5.018	537
500	-40.316	-45.880	-92.672	-8.783	-22.886	-26.130	-25.025	-2.139	900
1000	-17.292	-19.614	-43.056	-4.062	-10.062	-11.280	-10.221	-0.159	1800
1200	-13.414	-15.208	-34.754	-3.275	-7.899	-8.811	-7.764	+0.135	2160
1400	-10.630	-12.054	-28.812	-2.712	-6.347	-7.021	-6.014	+0.333	2520
1600	-8.532	-9.684	-24.350	-2.290	-5.180	-5.677	-4.706	+0.474	2880
1700	-7.666	-8.706	-22.512	-2.116	-4.699	-5.124	-4.169	+0.530	3060
1800	-6.896	-7.836	-20.874	-1.962	-4.270	-4.613	-3.693	+0.577	3240
1900	-6.204	-7.058	-19.410	-1.823	-3.886	-4.190	-3.267	+0.619	3420
2000	-5.580	-6.356	-18.092	-1.699	-3.540	-3.776	-2.884	+0.656	3600
2100	-5.016	-5.720	-16.898	-1.586	-3.227	-3.434	-2.539	+0.688	3780
2200	-4.502	-5.142	-15.810	-1.484	-2.942	-3.091	-2.226	+0.716	3960
2300	-4.032	-4.614	-14.818	-1.391	-2.682	-2.809	-1.940	+0.742	4140
2400	-3.600	-4.130	-13.908	-1.305	-2.443	-2.520	-1.679	+0.764	4320
2500	-3.202	-3.684	-13.070	-1.227	-2.224	-2.270	-1.440	+0.784	4500
2600	-2.836	-3.272	-12.298	-1.154	-2.021	-2.038	-1.219	+0.802	4680
2700	-2.494	-2.892	-11.580	-1.087	-1.833	-1.823	-1.015	+0.818	4860
2800	-2.178	-2.536	-10.914	-1.025	-1.658	-1.624	-0.825	+0.833	5040
2900	-1.882	-2.206	-10.294	-0.967	-1.495	-1.438	-0.649	+0.846	5220
3000	-1.606	-1.898	-9.716	-0.913	-1.343	-1.265	-0.485	+0.858	5400
3100	-1.348	-1.610	-9.174	-0.863	-1.201	-1.103	-0.332	+0.869	5580
3200	-1.106	-1.340	-8.664	-0.815	-1.067	-0.951	-0.189	+0.878	5760
3300	-0.878	-1.086	-8.186	-0.771	-0.942	-0.809	-0.054	+0.888	5940
3400	-0.664	-0.846	-7.736	-0.729	-0.824	-0.674	+0.071	+0.895	6120
3500	-0.462	-0.620	-7.312	-0.690	-0.712	-0.547	+0.190	+0.902	6300

Source: Based on data from the JANAF Thermochemical Tables, NSRDS-NBS-37, 1971.

(Table from M.J.Moran and H.N.Shapiro, Fundamentals of Engineering Thermodynamics, John Wiley & Sons, Inc, 5th ed., 2006)

Annex 2. Thermodynamic and transport properties of gases

Thermodynamic and transport properties of different gases are given below. Specifically: Argon (Ar), Carbon (C), Methane (CH₄), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen atom (H), Hydrogen (H₂), Water (H₂O), Peroxide (H₂O₂), Hydroperoxyl (HO₂), Nitrogen atom (N), Nitrogen (N₂), Nitrous oxide (N₂O), Nitrogen monoxide (NO), Nitrogen dioxide (NO₂), Oxygen atom (O), Oxygen (O₂), Hydroxyl (OH), Acetylene (C₂H₂), n-decane (C₁₀H₂₂).

General equations are given in terms of different coefficients. In all these equations, temperature is given in K. The universal gas constant ($\hat{R} = 8.31447 \text{ kJ/kmolK}$) and the gas constant ($R = \hat{R}/W$) are used in the thermodynamic properties.

Specific heat at constant pressure:

$$\frac{c_p}{R} = \frac{\hat{c}_p}{\hat{R}} = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4$$

Absolute enthalpy (formation enthalpy is included) at $p = p^0 = 1 \text{ atm}$:

$$\frac{h^o(T)}{RT} = \frac{\hat{h}^o(T)}{\hat{R}T} = a_0 + \frac{a_1}{2} T + \frac{a_2}{3} T^2 + \frac{a_3}{4} T^3 + \frac{a_4}{5} T^4 + \frac{a_5}{T}$$

Absolute entropy at $p = p^0 = 1 \text{ atm}$:

$$\frac{s^o(T)}{R} = \frac{\hat{s}^o(T)}{\hat{R}} = a_0 \ln(T) + a_1 T + \frac{a_2}{2} T^2 + \frac{a_3}{3} T^3 + \frac{a_4}{4} T^4 + a_5$$

Dynamic viscosity and thermal conductivity:

$$\mu \left(\frac{\text{kg}}{\text{m s}} \right) = e^{b_0 + b_1 \ln T + b_2 (\ln T)^2 + b_3 (\ln T)^3}; \quad \lambda \left(\frac{\text{W}}{\text{m K}} \right) = e^{c_0 + c_1 \ln T + c_2 (\ln T)^2 + c_3 (\ln T)^3}$$

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 JANAF³. Transport properties (μ and λ) from CHEMKIN⁴.

List of gases considered: Argon (Ar), Carbon (C), Methane (CH₄), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen atom (H), Hydrogen (H₂), Water (H₂O), Peroxide (H₂O₂), Hydroperoxyl (HO₂), Nitrogen atom (N), Nitrogen (N₂), Nitrous oxide (N₂O), Nitrogen monoxide (NO), Nitrogen dioxide (NO₂), Oxygen atom (O), Oxygen (O₂), Hydroxyl (OH), Acetylene (C₂H₂), n-decane (C₁₀H₂₂).

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			-0.7453750000e+03	
S	JANAF_S	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00			0.4366000000e+01	

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			-0.7453750000e+03	
S	JANAF_S	0.2500000000e+01	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00	0.0000000000e+00			0.4366000000e+01	

#-----

C Carbon

JANAF-CHEMKIN

MW 0.1201115036e+02

2

200.0 1000.0

³ 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/>

⁴ See the same website: <http://www.sandia.gov/HiTempThermo/chemkin.html>.

```

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  0.2665214460e-12
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

```

#-----

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

```

#-----

CO Carbon monoxide

JANAF-CHEMKIN

MW 0.2801055050e+02

2

200.0 1000.0

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 0.3579533470e+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

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

#-----

CO2 Carbon dioxide

JANAF-CHEMKIN

MW 0.4400995064e+02

2

200.0 1000.0

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 0.2356773520e+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

#-----

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

#-----

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

```

#-----

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

```

#-----

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

#-----

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

#-----

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

#-----

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
$c_{p,\text{gas}}$ (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