DIPPR (Design Institute for Physical Property Data) Physical Properties Database

Revised January 2007

This database contains 33 fixed-value properties and 15 temperature-dependent properties of approximately 1793 industrially important compounds. (Accessable only from the presentation computer in the 3rd floor computer room with IP address IP 150.250.102.72. This computer is the one with the phone next to it.)

From the third floor go to link: http://dippr.byu.edu/public/
user: rowanthermo
pswd: che&dippr

The numeric data in the DIPPR File consist of 29 single value property constants and 15 temperature-dependent properties. Regression equations and coefficients for temperature-dependent properties are also given for calculating additional property values. All of the data are searchable, including Regression Coefficients, percent error, and minimum/maximum temperature values.

If experimental data are not available, values are estimated when possible. Temperature-dependent correlation coefficients, applicable upper and lower temperature limits, and values computed at these limits are included for temperature-dependent properties.

Properties Included (1793 commercially important chemicals and substances):

Temperature Dependent Properties

Property	DIPPR ID	Units
Heat Capacity of Ideal Gas	ICP	J/(kmol·K)
Heat Capacity of Liquid	LCP	J/(kmol·K)
Heat Capacity of Solid	SCP	J/(kmol·K)
Heat of Vaporization	HVP	J/kmol
Liquid Density	LDN	kmol/m³
Second Virial Coefficient	SVR	m³/kmol
Solid Density	SDN	kmol/m³
Surface Tension	ST	N/m
Thermal Conductivity of Liquid	LTC	W/(m·K)
Thermal Conductivity of Solid	STC	W/(m·K)
Thermal Conductivity of Vapor	VTC	W/(m·K)
Vapor Pressure of Liquid	VP	Pa
Vapor Pressure of Solid or Sublimation Pressure	SVP	Pa
Viscosity of Liquid	LVS	Pa·s

Viscosity of Vapor	VVS	Pa·s

Constant Property	**DIPPR ID**	**Units**
Acentric Factor	ACEN	---
Auto Ignition Temperature	AIT	K
Dipole Moment	DM	C·m
Absolute Entropy of Ideal Gas at 298.15 K and 1 bar	ENT	J/(kmol·K)
Lower Flammability Limit Temperature	FLTL	K
Upper Flammability Limit Temperature	FLTU	K
Lower Flammability Limit Percent	FLVL	Vol % in air
Upper Flammability Limit Percent	FLVU	Vol % in air
Flash Point	FP	K
Gibbs Energy of Formation for Ideal Gas at 298.15 K and 1 bar	**GFOR**	**J/kmol**
Standard State Gibbs Energy of Formation at 298.15 K and 1 bar	**GSTD**	**J/kmol**
Net Standard State Enthalpy of Combustion at 298.15 K	HCOM	J/kmol
Enthalpy of Formation for Ideal Gas at 298.15 K	**HFOR**	**J/kmol**
Enthalpy of Fusion at Melting Point	HFUS	J/kmol
Standard State Enthalpy of Formation at 298.15 K and 1 bar	**HSTD**	**J/kmol**
Heat of Sublimation	HSUB	J/kmol
Liquid Molar Volume at 298.15 K	LVOL	m^3/kmol
Melting Point at 1 atm	MP	K
Molecular Weight	MW	kg/kmol
Normal Boiling Point	NBP	K
Parachor	PAR	---
Critical Pressure	PC	Pa
Radius of Gyration	RG	m
Refractive Index	RI	---
Solubility Parameter at 298.15 K	SOLP	$(J/m^3)^{1/2}$
Standard State Absolute Entropy at 298.15 K and 1 bar	SSTD	J/(kmol·K)
Critical Temperature	TC	K
Triple Point Pressure	TPP	Pa
Triple Point Temperature	TPT	K
Critical Volume	VC	m^3/kmol
van der Waals Area	VDWA	m^2/kmol
van der Waals Reduced Volume	VDWV	m^3/kmol

Critical Compressibility Factor	ZC	---

Integrating DIPPR Heat Capacities
Ideal Gas Heat Capacity is given as:

$$C_{pi} = A + B\left[\frac{C/T}{\sinh(C/T)}\right]^2 + D\left[\frac{E/T}{\cosh(E/T)}\right]^2 \quad \text{with T in Kelvin and Cp [=] J/kmol*K}$$

$$\Delta H = \int C_p \mathrm{d}T = A\Delta T + BC\left[\coth(C/T_2) - \coth(C/T_1)\right] - DE\left[\tanh(E/T_2) - \tanh(E/T_1)\right]$$

Remember that the enthalpy of a gas is calculated from its standard state enthalpy (See equation 8-19 in Fogler 4th ed. on page 482.)

Below is an example of calculating heat capacities and average heat capacities using DIPPR values for oxygen.

Oxygen Heat Capacities Values
The table below gives a summary of the constant property values that are independent of temperature. You will need the Ideal Gas Heat of Formation for an enthalpy calculation.

Address http://dippr.byu.edu/public/chemsearch.asp?Mode=Printout1&ChemID=901

Chemical Database Property Constants

UNITS | TEMPERATURE DEPENDENT | PROPERTY CALCULATOR | NEW SEARCH | LINKS | FEEDBACK

Chemical Abstracts Name:oxygen — O_2
IUPAC Name:oxygen — oxygen
Synonym: refrigerant 732
Chemical Abstracts Number*: 7782-44-7 — Structural Formula: O_2

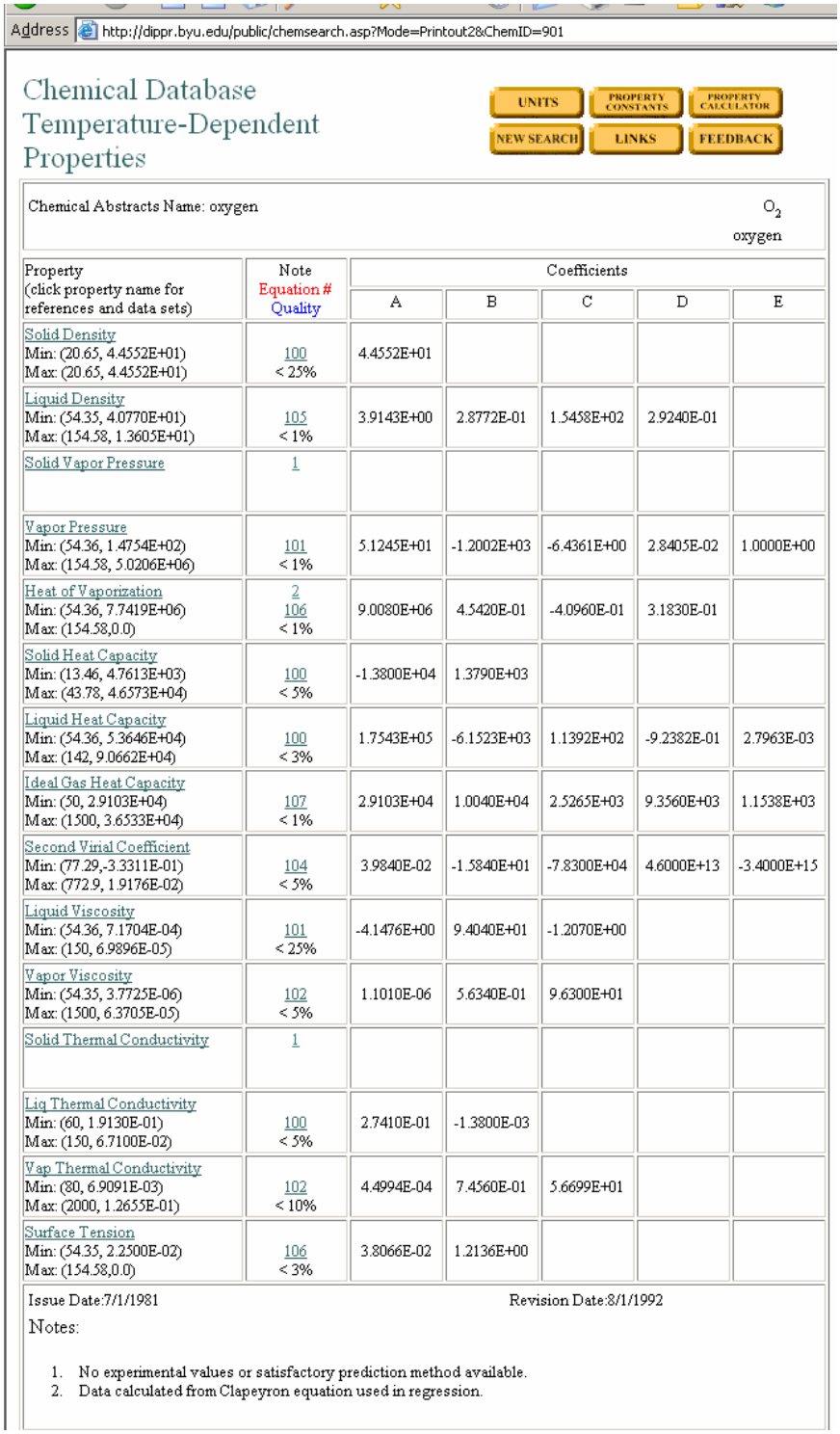
Property (click property name for references and data)	Units	Value	Note	Quality Code: Data type	Quality Code: Reliability	Quality Code: Source type
Molecular Weight	kg/kmol	31.9988				
Critical Temperature	K	154.58		Experimental	< 3%	Evaluated
Critical Pressure	Pa	5.04300E+06		Experimental	< 5%	Evaluated
Critical Volume	m^3/kmol	7.34000E-02		Experimental	< 10%	Evaluated
Crit Compress Factor	unitless	0.288		Defined	None	Staff
Melting Point	K	54.361	1	Experimental	< 1%	Evaluated
Triple Pt Temperature	K	54.361		Experimental	< 1%	Evaluated
Triple Pt Pressure	Pa	150		Experimental	< 3%	Evaluated
Normal Boiling Point	K	90.188		Experimental	< 1%	Evaluated
Liq Molar Volume	m^3/kmol	2.80225E-02	2	Experimental	< 1%	Staff
IG Heat of Formation	J/kmol	0.0				
IG Gibbs of Formation	J/kmol	0.0				
IG Absolute Entropy	J/kmol*K	2.05043E+05		Experimental	< 0.2%	Evaluated
Std Heat of Formation	J/kmol	0.0				
Std Gibbs of Formation	J/kmol	0.0	3	Defined	Unknown	Staff
Std Absolute Entropy	J/kmol*K	2.05043E+05		Experimental	< 0.2%	Evaluated
Heat Fusion at Melt Pt	J/kmol	4.44000E+05		Experimental	< 3%	Evaluated
Std Net Heat of Comb	J/kmol	0.0				
Acentric Factor	unitless	2.21798E-02		Defined	None	Staff
Radius of Gyration	m	6.80000E-11		Defined	< 3%	Staff
Solubility Parameter	(J/m^3)^0.5	8.18200E+03	4	Defined	None	Staff
Dipole Moment	c*m	0.0				
van der Waals Volume	m^3/kmol	1.30000E-02		Defined	< 3%	Staff
van der Waals Area	m^2	2.35000E+08	5	Defined	< 5%	Staff
Refractive Index	unitless	1.221	6	Experimental	Unknown	Evaluated
Flash Point	K		7			
Lower Flammability Limit	vol% in air		7			
Upper Flammability Limit	vol% in air		7			
Lower Flamm Limit Temp	K					
Upper Flamm Limit Temp	K					
Auto Ignition Temp	K		7			
Parachor	unitless					
Heat of Sublimation	J/kmol					
Dielectric Constant	unitless					

Issue Date: 7/1/1981 — Revision Date: 8/1/1994

Notes:

1. Triple point temperature.
2. Determined at the normal boiling point.
3. Calculated from the standard state enthalpy of formation and the standard state absolute entropy.
4. For the hypothetical liquid at 298 K and 101325 Pa.

Below is the page showing the temperature Dependent properties.



Address http://dippr.byu.edu/public/chemsearch.asp?Mode=Printout2&ChemID=901

Chemical Database Temperature-Dependent Properties

UNITS | PROPERTY CONSTANTS | PROPERTY CALCULATOR | NEW SEARCH | LINKS | FEEDBACK

Chemical Abstracts Name: oxygen O_2 oxygen

Property (click property name for references and data sets)	Note Equation # Quality	Coefficients A	B	C	D	E
Solid Density Min: (20.65, 4.4552E+01) Max: (20.65, 4.4552E+01)	100 < 25%	4.4552E+01				
Liquid Density Min: (54.35, 4.0770E+01) Max: (154.58, 1.3605E+01)	105 < 1%	3.9143E+00	2.8772E-01	1.5458E+02	2.9240E-01	
Solid Vapor Pressure	1					
Vapor Pressure Min: (54.36, 1.4754E+02) Max: (154.58, 5.0206E+06)	101 < 1%	5.1245E+01	-1.2002E+03	-6.4361E+00	2.8405E-02	1.0000E+00
Heat of Vaporization Min: (54.36, 7.7419E+06) Max: (154.58,0.0)	2 106 < 1%	9.0080E+06	4.5420E-01	-4.0960E-01	3.1830E-01	
Solid Heat Capacity Min: (13.46, 4.7613E+03) Max: (43.78, 4.6573E+04)	100 < 5%	-1.3800E+04	1.3790E+03			
Liquid Heat Capacity Min: (54.36, 5.3646E+04) Max: (142, 9.0662E+04)	100 < 3%	1.7543E+05	-6.1523E+03	1.1392E+02	-9.2382E-01	2.7963E-03
Ideal Gas Heat Capacity Min: (50, 2.9103E+04) Max: (1500, 3.6533E+04)	107 < 1%	2.9103E+04	1.0040E+04	2.5265E+03	9.3560E+03	1.1538E+03
Second Virial Coefficient Min: (77.29,-3.3311E-01) Max: (772.9, 1.9176E-02)	104 < 5%	3.9840E-02	-1.5840E+01	-7.8300E+04	4.6000E+13	-3.4000E+15
Liquid Viscosity Min: (54.36, 7.1704E-04) Max: (150, 6.9896E-05)	101 < 25%	-4.1476E+00	9.4040E+01	-1.2070E+00		
Vapor Viscosity Min: (54.35, 3.7725E-06) Max: (1500, 6.3705E-05)	102 < 5%	1.1010E-06	5.6340E-01	9.6300E+01		
Solid Thermal Conductivity	1					
Liq Thermal Conductivity Min: (60, 1.9130E-01) Max: (150, 6.7100E-02)	100 < 5%	2.7410E-01	-1.3800E-03			
Vap Thermal Conductivity Min: (80, 6.9091E-03) Max: (2000, 1.2655E-01)	102 < 10%	4.4994E-04	7.4560E-01	5.6699E+01		
Surface Tension Min: (54.35, 2.2500E-02) Max: (154.58,0.0)	106 < 3%	3.8066E-02	1.2136E+00			

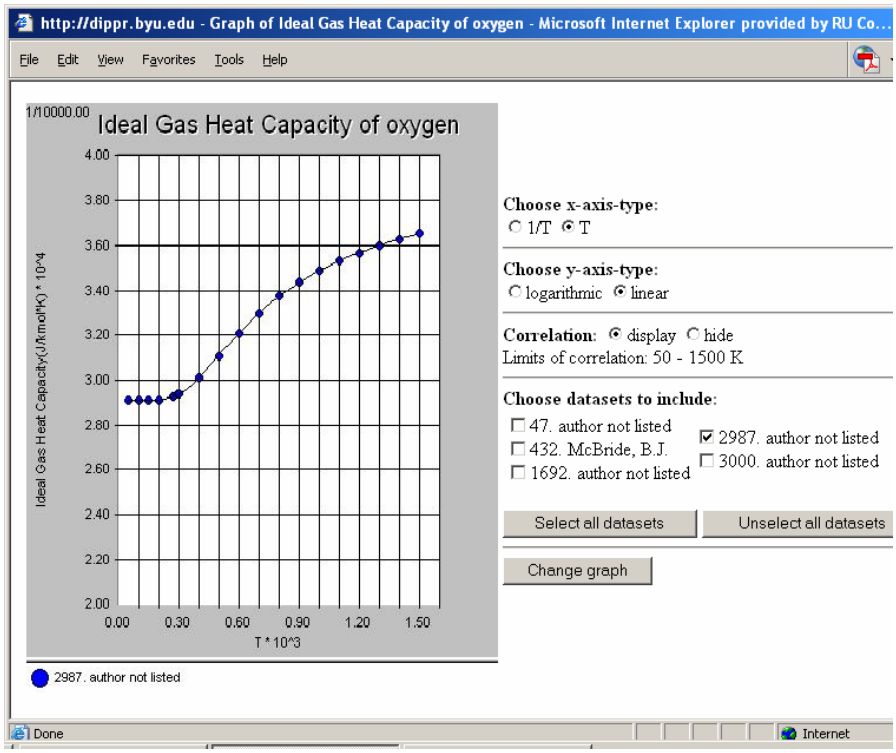
Issue Date:7/1/1981 Revision Date:8/1/1992

Notes:

1. No experimental values or satisfactory prediction method available.
2. Data calculated from Clapeyron equation used in regression.

http://dippr.byu.edu/public/chemsearch.asp?Mode=Reference&ChemID=901&Property=ICP

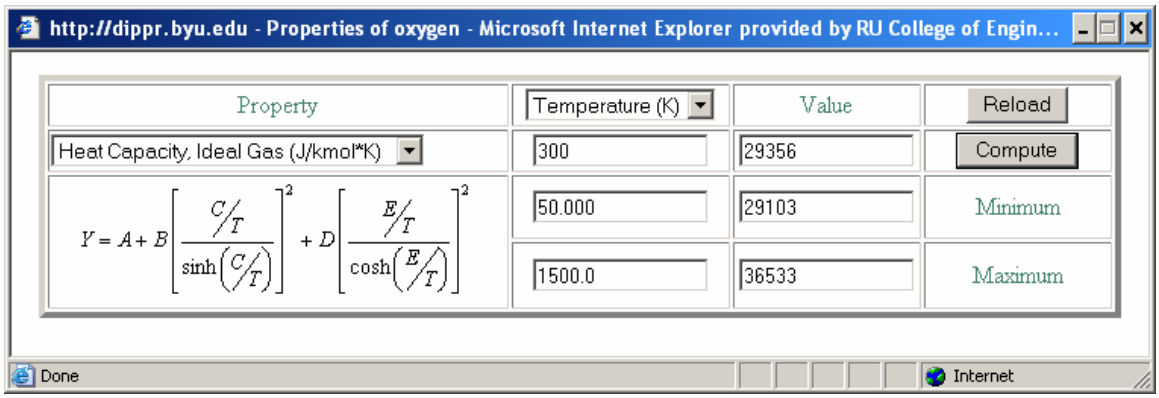
From the Property Calculator:



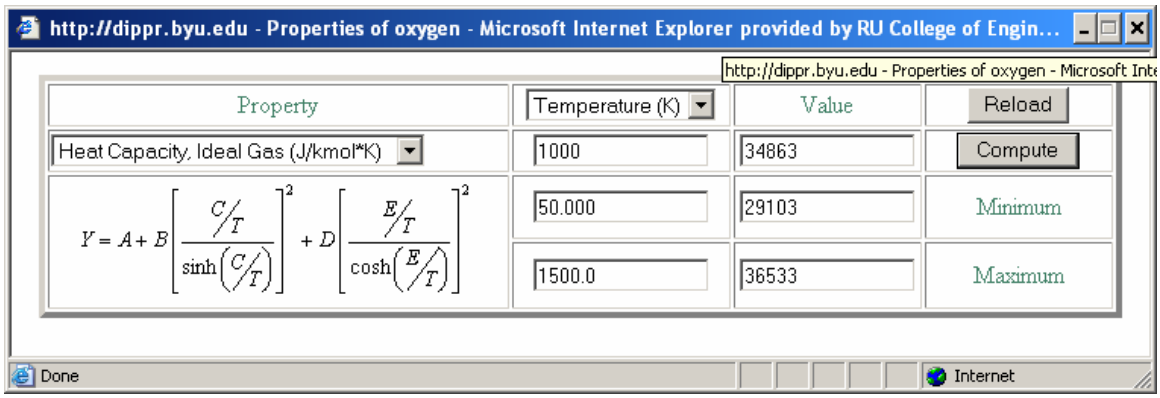
2987. *TRC Thermodynamic Tables-Hydrocarbons*; Thermodynamics Research Center, The Texas A&M University System, College Station, TX, **1985**.

Temperature (K)	Ideal Gas Heat Capacity (J/kmol*K)
50	**2.91030E+04**
100	**2.91060E+04**
150	**2.91090E+04**
200	**2.91260E+04**
273.16	**2.92720E+04**
298.15	**2.93760E+04**
300	**2.93850E+04**
400	**3.01060E+04**
500	**3.10910E+04**
600	**3.20900E+04**
700	**3.29810E+04**
800	**3.37330E+04**
900	**3.43550E+04**
1000	**3.48700E+04**
1100	**3.53000E+04**
1200	**3.56670E+04**
1300	**3.59880E+04**
1400	**3.62770E+04**
1500	**3.65440E+04**

Here are the fitted values of Heat Capacity for oxygen gas at temperatures of 300K and 1000K. Notice that these are not the average heat capacities for the range of 300 to 1000K.



To



calculate the average heat capacity value from DIPPR constants POLYMATH can be used to numerically integrate – or to check you analytical integration. For Example from the result below the value of the average heat capacity for oxygen from 300 K to 1000 K is 3.235×10^4 J/(kmol K). This result can also be obtained from a numerical integration.

$$C_{pi} = A + B\left[\frac{C/T}{\sinh(C/T)}\right]^2 + D\left[\frac{E/T}{\cosh(E/T)}\right]^2 \quad \text{with T in Kelvin and Cp [=] J/kmol*K}$$

$$\Delta H = \int_{300K}^{1000K} C_p dT = A(1000-300) + BC\left[\coth(C/1000K) - \coth(C/300K)\right] - DE\left[\tanh(E/1000K) - \tanh(E/300K)\right]$$

$$\overline{C}_p = \frac{\int_{300K}^{1000k} C_p dT}{1000K - 300K} = 3.235\times10^4 \text{ J/(kmol K)}$$

This is given as the final value of Cpavg in the POLYMATH program given below.

For a numerical integration Polymath can be used:

POLYMATH Report oxygen heat capacity 2006
Ordinary Differential Equations 23-Jan-2006

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	T	298.	298.	1000.	1000.
2	H	0	0	2.27E+07	2.27E+07
3	A	2.91E+04	2.91E+04	2.91E+04	2.91E+04
4	B	1.004E+04	1.004E+04	1.004E+04	1.004E+04
5	C	2526.5	2526.5	2526.5	2526.5
6	D	9356.	9356.	9356.	9356.
7	E	1153.8	1153.8	1153.8	1153.8
8	Cp	2.935E+04	2.935E+04	3.486E+04	3.486E+04
9	**Cpavg**	0	0	3.235E+04	**3.235E+04**

Differential equations

1 d(H)/d(T) = Cp

Explicit equations

1 A = 2.9103e4

2 B = 1.0040e4

3 C = 2526.5

4 D = 9.3560e3

5 E = 1.1538e3

6 Cp = A + B * (C / T / sinh(C / T)) ^ 2 + D * (E / T / cosh(E / T)) ^ 2

7 Cpavg = H / (1000 - 300)

General

Total number of equations	8
Number of differential equations	1
Number of explicit equations	7
Elapsed time	0.000 sec
Solution method	RKF_45
Step size guess. h	0.000001
Truncation error tolerance. eps	0.000001

Note you can change the units of your system on this page: