

Oxygen

Other names:	Dioxygen Liquid oxygen Molecular oxygen O2 Oxygen molecule Pure oxygen UN 1072 UN 1073
Inchi:	InChI=1S/O2/c1-2
InchiKey:	MYMOFIZGZYHOMD-UHFFFAOYSA-N
Formula:	O2
SMILES:	O=O
Mol. weight [g/mol]:	32.00
CAS:	7782-44-7

Physical Properties

Property code	Value	Unit	Source
af	0.0250		KDB
affp	421.00 ± 3.00	kJ/mol	NIST Webbook
affp	421.00	kJ/mol	NIST Webbook
basg	396.30	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
ea	1.10 ± 0.10	eV	NIST Webbook
ea	0.45 ± 0.01	eV	NIST Webbook
ea	0.45 ± 0.02	eV	NIST Webbook
ea	0.73	eV	NIST Webbook
ea	1.27 ± 0.20	eV	NIST Webbook
ea	0.56 ± 0.10	eV	NIST Webbook
ea	0.48	eV	NIST Webbook
ea	0.15 ± 0.05	eV	NIST Webbook
ea	0.45 ± 0.01	eV	NIST Webbook
ea	0.44 ± 0.01	eV	NIST Webbook
ea	0.45 ± 0.10	eV	NIST Webbook
ea	0.44 ± 0.10	eV	NIST Webbook
ea	0.40 ± 0.10	eV	NIST Webbook
ea	0.43 ± 0.02	eV	NIST Webbook
ea	0.50 ± 0.10	eV	NIST Webbook

ea	0.43 ± 0.03	eV	NIST Webbook
ea	0.46 ± 0.05	eV	NIST Webbook
ea	0.45 ± 0.05	eV	NIST Webbook
ea	0.50 ± 0.20	eV	NIST Webbook
ea	1.12 ± 0.07	eV	NIST Webbook
gf	-447.78	kJ/mol	Joback Method
gyrad	0.6040		KDB
hf	-426.93	kJ/mol	Joback Method
hfus	6.37	kJ/mol	Joback Method
hvap	27.12	kJ/mol	Joback Method
ie	12.06 ± 0.00	eV	NIST Webbook
ie	12.20 ± 0.20	eV	NIST Webbook
ie	12.06 ± 0.00	eV	NIST Webbook
ie	12.08 ± 0.01	eV	NIST Webbook
ie	12.07 ± 0.01	eV	NIST Webbook
ie	12.13	eV	NIST Webbook
ie	12.08 ± 0.01	eV	NIST Webbook
ie	12.00 ± 0.50	eV	NIST Webbook
ie	12.08	eV	NIST Webbook
ie	12.08	eV	NIST Webbook
ie	12.30	eV	NIST Webbook
ie	12.07 ± 0.00	eV	NIST Webbook
ie	12.07 ± 0.00	eV	NIST Webbook
ie	12.33 ± 0.01	eV	NIST Webbook
ie	12.80 ± 0.50	eV	NIST Webbook
ie	12.00 ± 1.00	eV	NIST Webbook
ie	12.07 ± 0.01	eV	NIST Webbook
ie	12.07	eV	NIST Webbook
ie	12.07 ± 0.00	eV	NIST Webbook
ie	12.10 ± 0.10	eV	NIST Webbook
ie	12.08 ± 0.00	eV	NIST Webbook
log10ws	-0.95		Crippen Method
logp	0.067		Crippen Method
mcvol	18.300	ml/mol	McGowan Method
pc	4985.19 ± 30.39	kPa	NIST Webbook
pc	4992.28 ± 30.39	kPa	NIST Webbook
pc	5043.00 ± 0.50	kPa	NIST Webbook
pc	5003.43 ± 30.39	kPa	NIST Webbook
pc	5043.00	kPa	KDB
pt	0.15	kPa	KDB
rhoc	435.18 ± 0.45	kg/m3	NIST Webbook
sgb	205.15 ± 0.01	J/mol×K	NIST Webbook
tb	90.20 ± 0.20	K	NIST Webbook
tb	90.20	K	KDB

tc	154.59	K	KDB
tc	154.58 ± 0.00	K	NIST Webbook
tc	154.58 ± 0.00	K	NIST Webbook
tc	155.15 ± 0.30	K	NIST Webbook
tf	54.80 ± 0.20	K	NIST Webbook
tf	54.36	K	KDB
tt	54.33 ± 0.06	K	NIST Webbook
tt	54.36	K	KDB
vc	0.073	m3/kmol	KDB
zc	0.2864140		KDB
zra	0.29		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	21.37	J/mol×K	289.79	Joback Method
cpg	11.77	J/mol×K	195.80	Joback Method
cpg	14.04	J/mol×K	214.60	Joback Method
cpg	16.12	J/mol×K	233.40	Joback Method
cpg	18.04	J/mol×K	252.20	Joback Method
cpg	19.78	J/mol×K	270.99	Joback Method
cpg	9.31	J/mol×K	177.00	Joback Method
dvisc	0.0114021	Pa×s	126.66	Joback Method
dvisc	0.0078823	Pa×s	135.05	Joback Method
dvisc	0.0056896	Pa×s	143.44	Joback Method
dvisc	0.0042575	Pa×s	151.83	Joback Method
dvisc	0.0032841	Pa×s	160.22	Joback Method
dvisc	0.0021038	Pa×s	177.00	Joback Method
dvisc	0.0025996	Pa×s	168.61	Joback Method
hvapt	9.26	kJ/mol	30.50	Measurements of enthalpy of sublimation of Ne, N2, O2, Ar, CO2, Kr, Xe, and H2O using a double paddle oscillator
rhoI	1149.00	kg/m3	90.00	KDB
srf	0.02	N/m	80.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension

srf	0.01	N/m	90.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension
srf	0.01	N/m	100.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension
srf	0.01	N/m	115.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension
srf	0.01	N/m	120.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension
srf	0.01	N/m	124.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension
srf	0.00	N/m	128.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension
srf	0.00	N/m	132.00	The liquid gas interface of oxygen nitrogen solutions 1. Surface tension

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37279e+01
Coeff. B	-7.81059e+02
Coeff. C	-4.45000e+00
Temperature range (K), min.	54.35
Temperature range (K), max.	154.58

Datasets

Speed of sound, m/s

Temperature, K - Fluid (supercritical or subcritical phases)	Pressure, kPa - Fluid (supercritical or subcritical phases)	Speed of sound, m/s - Fluid (supercritical or subcritical phases)
499.03	4920.00	434.71
399.09	4960.00	388.03
499.03	5910.00	436.52
449.94	6010.00	414.33
399.09	6020.00	389.77
499.03	7820.00	440.23
399.09	7950.00	393.26
449.95	8010.00	418.16
349.98	8030.00	367.01
299.97	9920.00	340.22
449.94	9970.00	422.01
399.11	9980.00	397.34
498.94	10000.00	444.64
349.99	10070.00	370.9
299.96	14860.00	352.65
499.02	14940.00	455.31
349.99	14980.00	382.53
449.94	15000.00	433.26
399.10	15010.00	408.72
349.99	19640.00	396.03
399.06	19900.00	421.58
449.94	20010.00	445.6
299.97	20050.00	370.99
499.04	20070.00	467.39
499.01	24900.00	479.52
449.94	24940.00	458.85
349.99	24980.00	414.2
399.09	25010.00	436.72
299.97	25030.00	392.82
399.09	29900.00	452.47
499.00	29910.00	492.81
299.97	29960.00	417.33
349.98	29990.00	433.29

449.94	30000.00	473.4
499.00	34730.00	506.11
399.08	34890.00	469.6
299.97	34960.00	443.87
449.93	35030.00	488.6
349.99	35080.00	454.09
299.97	39960.00	471.2
399.08	39970.00	487.82
498.99	40010.00	521.13
449.93	40050.00	504.35
350.03	40050.00	475.39
499.00	44900.00	535.41
399.08	44980.00	506.29
349.99	45020.00	497.15
299.97	45030.00	498.92
449.94	45090.00	520.58
349.98	49900.00	518.73
449.94	49910.00	536.52
499.03	49930.00	550.29
299.97	50010.00	525.82
399.09	50090.00	525.43
499.03	54810.00	564.89
399.08	54970.00	543.88
449.90	55090.00	553.54
349.99	55110.00	541.66
299.97	55140.00	552.86
349.99	59910.00	562.59
498.89	60010.00	580.54
449.90	60070.00	570.12
399.08	60070.00	563.14
299.97	60160.00	578.47
399.08	64900.00	581.28
350.03	64930.00	584.11
299.97	64960.00	602.28
498.89	65000.00	595.63
449.89	65180.00	587.16
349.99	68690.00	600.07
299.97	69690.00	624.95
498.83	69940.00	610.55
399.08	70100.00	600.65
449.89	70120.00	603.58
300.00	74030.00	645.07
399.07	74590.00	617.2
498.91	74960.00	625.69

449.88	75270.00	620.61
349.98	78850.00	641.85
399.07	79990.00	636.78
498.92	79990.00	640.74
449.87	80010.00	636.12
399.05	83180.00	648.15
498.93	84890.00	655.27
449.88	85020.00	652.33
449.79	87520.00	660.32
449.95	88050.00	662.01
498.91	90000.00	670.28
498.90	95000.00	684.96
498.91	100060.00	699.53

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Abstract

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Solubilities of CO₂, H₂, N₂ and O₂ in ionic liquid
Thermodynamic properties of 4-bromobutyrate:
Energetics of neutral and deprotonated (Z)-cinnamic acid:
A calorimetric and thermodynamic investigation of zinc and cadmium complexes and computational study of (1H-Indol-3-yl)methanol and 2-ethyl-1H-imidazole (N-2,2'-bis(N,N-diethylthioureas):
Investigation in the variation of Gibbs energy of formation of RE₂UO₂12 (RE = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Y, Yb, Lu, Sc, Th, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr) system and the stability functions of Magnesium-ammonium hydrogen phosphate hold hands: The thermochemistry of thermodynamic properties of alkyl 1H-indole carboxylate derivatives: A combined experimental and oxygen nitrogen solutions: Surface tension: Thermochemistry of ammonium based ionic liquids: Tetra-alkyl-ammonium fluoride complex formation and optimization of pressure-temperature measurements of binary mixtures rich in low temperature applications and the Standard Molar Enthalpy of Formation Solubilities of several binary gases in 1,2-bis(2-aziridinyl)ethane and 1,2-bis(2-aziridinyl)ethane: 2,2,2-trifluoroethyl formate 298.15 K and 400 K: Coumarin: Thermochemical and thermophysical study of 2-thiophenecarboxylic acid: Furanose and 2-thiophenecarboxylic acid: Thermodynamics of the Guerbet condensation of 2-ethyl-3-coumaranone isomers: A combined calorimetric and computational study:

Determination of the energies of combustion and enthalpies of formation of 1,2-dichloroethane and 1,1,2-trichloroethane and of pyrene in cyclohexane by experiment and molecular thermodynamic study of two polymethylpyrazine N,N-dioxide: Experimental and computational thermochemical studies of acridone: Thermodynamic properties of rare earth complexes with salicylic acid: Benchmark properties of diphenyl oxide as a potential liquid organic polymer carrier: Evaluation of computational study of the energetics of 1,2-dichloroethane: Experimental and computational study of the molecular energetics of the three monofluorobenzene isomers: Thermochemical Properties of Formamide Revisited: New Experiment and computational study of formation of copper(II) beta-diketonates and thermodynamic properties of 1-Butyl-3-Methylimidazolium Nitrate: Thermochemical study of three dibromophenol isomers: Experimental and computational thermochemical studies of 5-methyl-2-thiophenecarboxylic acid: Thermodynamic properties of 1,4-benzodioxan and 1,4-dioxane: Thermochemical study of 9-anthracenecarboxylic acid: Experimental and computational study on the molecular energetics of 9-anthracenecarboxylic acid and ethyl 2-thiophenecarboxylates and ethyl 2-thiophenecarboxylates: solvent-free reaction between
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Benchmark thermodynamic properties of 1,3-propanediol: Comprehensive experimental and theoretical study: FORMATION OF L-ASPARAGINE AND EXPERIMENTAL THERMOCHEMICAL STUDY OF 2,5- AND 2,6-DICHLORO-4-NITROANILINES: Experimental and theoretical study of methyl n-hydroxybenzoates: Standard molar enthalpies of formation in the crystalline phase of 5-oxo-2-pentanone: Thermodynamic Properties of FOX-7 and Its Five Closed-Loop Isomers: Experimental and computational thermochemical studies of benzoxazole and methoxycarbonyl oxazole revisited: Solubility of oxygen in substituted perfluorocarbons: Experimental and computational energetic study of 1-R-2-phenylindole: Experimental and computational study of the energetics of 5- and 6-methyluracil and second virial cross coefficient of water + oxygen and water solubility (CO₂, O₂, Ar, N₂, H₂, and He) in Liquid Chlorinated Methanes: Thermodynamic properties of methylprednisolone aceponate: Thermodynamic and aromaticity studies for the assessment of the halogen-exchange interactions on investigation on the thermochemistry of orthophenylpyrroles: Enthalpy of oxygen carriers for biomass gasification: Combustion - thermodynamic data: Experimental and computational enthalpies and Gibbs energies of formation and binary vapor-liquid Equilibrium Data for Perfluoropropane with Light Gases (Oxygen, Nitrogen, and Methane) stereoisomers: Solubilities of Gases in 1,1,3,3-Tetramethylguanidium Lactate at Elevated Pressure: Stability of the three isomers of methoxybenzamide: Thermodynamic properties of pyruvic acid and its methyl ester: Enthalpy of formation of 5-fluoro-1,3-dimethyluracil: Spectroscopy and Calorimetric, Thermodynamic, Spectroscopic, and Computational Investigations of CO₂-based binary systems containing N₂, O₂ and Ar: Experimental measurements and theoretical results with advanced cubic equations of state: Experimental and computational thermochemical study of two fluoropropanes: computational study of the thermodynamic properties of 2-hydroxy-2-methyl-2-phenylaziridine: thermodynamic study: Determination of Dichlorodifluoromethane's Diffusion Coefficients in Hydrogen, Helium, Nitrogen, Boron Trifluoride, Flow Evaporation, and Formation of the Mn₂-xO₄ (x=0.05-0.1) spinel phase: molar enthalpy of formation of methoxyacetophenone isomers: Selective adsorption of CO₂ from H₂, O₂ and N₂ by 5-methyl-6-methyluracil: Enthalpies of formation of hydroxyalcohol and fluoromethacrylate Synthesis, structure, and thermodynamics of a lanthanide energetic structural effects of amino acid moieties in the thermodynamic study of 5-methyluracil, 6-methyluracil, and 5-methyluracil: Experimental and computational study of the gas-phase thermochemistry of formation: 1-phenylhydrazine and tetraphenylantimony benzoate and tetraphenylantimony benzoate: Ph₄SbOC(O)Ph:

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Measurements of the Calorific Value of Methane with the New GERG Reference Equation and molecular structure of alkyl 1-methylpyrrolocarboxylates (Santunien, Myrberg, and reactivity properties of phenoxazine and Experimental and computational study of the energetics of hydantoin and Experimental thermochemical study of 4,5-dichloro-2-nitroaniline: Equilibrium Data for the Oxygen + Propane Binary System at Temperatures of 1100, 1200, 1300, 1400, and 1500 K; Benzonitrile and Benzoylbenzoin stability of Ca3TeO6 determined by a solid electrolyte EMF Standard molar enthalpies of formation and of sublimation of the terphenyl isomers of the Single Gases Carbon Monoxide and Oxygen in the Ionic Thermodynamic Properties of three-ring aza-aromatics. 1. Thermodynamic Properties for 2,4,6-trimethyl-1,3,5-triazine and 2,4,6-trimethyl-1,3,5-triazine-2-thione and 2,4,6-trimethyl-1,3,5-triazine-2-thione: A thermodynamic study of some dihydroresorcinol isomers of dihydroresorcinol isomers: Structural studies of cyclic ureas: 3. Enthalpy of formation of barbital: KDB:

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3-methyl-2-cyclopentenone: Structure and energetics correlations in some chlorohydroxypyridines:

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Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density

rho:	Liquid Density
sgb:	Molar entropy at standard conditions (1 bar)
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter

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