Diborane

Other names:	B2H6
	Boroethane
	Boron hydride
	Boron hydride (B2H6)
	Diborane(6)
	Diboron hexahydride
	UN 1911
Inchi:	InChI=1S/B2H2/c1-3-2-4-1
InchiKey:	GCXMMZWJUYHRTG-UHFFFAOYSA-N
Formula:	B2H6
Mol. weight [g/mol]:	27.67
CAS:	19287-45-7

Physical Properties

Property code	Value	Unit	Source
affp	615.00	kJ/mol	NIST Webbook; Hunter and Lias, 1998
basg	586.00	kJ/mol	NIST Webbook; Hunter and Lias, 1998
ie	11.90	eV	NIST Webbook; Asbrink, Svensson, et al., 1981
ie	11.37 ± 0.05	eV	NIST Webbook; Ruscic, Mayhew, et al., 1988
ie	11.41 ± 0.02	eV	NIST Webbook; Lloyd and Lynaugh, 1970
ie	11.38 ± 0.01	eV	NIST Webbook; Brundle, Robin, et al., 1970
ie	20.20 ± 0.10	eV	NIST Webbook; Brundle, Robin, et al., 1970
ie	11.37 ± 0.01	eV	NIST Webbook; Rose, Frey, et al., ibid.
ie	11.38 ± 0.05	eV	NIST Webbook; N/A
ie	11.40	eV	NIST Webbook; Asbrink, Svensson, et al., 1981
pc	4053.00	kPa	Mathews (1972), critical constants of inorganic substances
pc	4053.00	kPa	Air Liquide Gas Encyclopedia
tb	180.65	K	Air Liquide Gas Encyclopedia

tc	289.80	K	Mathews (1972), critical constants of inorganic substances
tc	289.80	K	Air Liquide Gas Encyclopedia
tt	108.32	K	Staveley, Lobo and Calado (1981), triple points

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	14.26	kJ/mol	180.65	Air Liquide Gas Encyclopedia
hvapt	15.30	kJ/mol	148.50	NIST Webbook; Ditter, Perrine, et al., 1961
hvapt	14.20	kJ/mol	180.00	NIST Webbook; Paridon, MacWood, et al., 1959
hvapt	12.60	kJ/mol	210.00	NIST Webbook; Paridon, MacWood, et al., 1959
hvapt	10.50	kJ/mol	240.00	NIST Webbook; Paridon, MacWood, et al., 1959
hvapt	7.30	kJ/mol	270.00	NIST Webbook; Paridon, MacWood, et al., 1959
rhog	1.92	kg/m3	180.65	Air Liquide Gas Encyclopedia
rhog	1.18	kg/m3	288.15	Air Liquide Gas Encyclopedia
rhol	421.00	kg/m3	180.65	Air Liquide Gas Encyclopedia

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot t + C \cdot t^2 + D \cdot t^3 + E/t^2$, $t = T/1000$
Y unit	J/mol×K

Coeff. A	-1.24217e+01
Coeff. B	2.67611e+02
Coeff. C	-1.52261e+02
Coeff. D	3.31588e+01
Coeff. E	3.00489e-01
Reference	Chase, 1998
Comment	F=35.09886, G=146.5115, H=41.00303; Data last reviewed in December, 1964
Temperature range (K), min.	298.00
Temperature range (K), max.	1200.00

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot t + C \cdot t^2 + D \cdot t^3 + E/t^2$, $t = T/1000$
Y unit	J/mol×K
Coeff. A	1.61627e+02
Coeff. B	1.12333e+01
Coeff. C	-2.17819e+00
Coeff. D	1.46029e-01
Coeff. E	-3.67676e+01
Reference	Chase, 1998
Comment	F=-89.40873, G=320.5023, H=41.00303; Data last reviewed in December, 1964
Temperature range (K), min.	1200.00
Temperature range (K), max.	6000.00

Information	Value
Property code	pvap
Equation	$\ln(Y) = A + B/(T + C)$
Y unit	kPa
Coeff. A	1.37235e+01
Coeff. B	-1.50665e+03
Coeff. C	-1.51800e+01
Temperature range (K), min.	107.65
Temperature range (K), max.	289.80

Information	Value
Property code	pvap
Equation	$\ln(Y) = A + B/(T + C)$
Y unit	kPa
Coeff. A	1.33125e+01
Coeff. B	-1.37784e+03

Coeff. C	-2.21750e+01
Reference	Ditter, Perrine, et al., 1961, 2
Comment	Coefficents calculated by NIST from author's data.
Temperature range (K), min.	118.30
Temperature range (K), max.	180.80

Information	Value
Property code	pvap
Equation	ln(Y) = A + B/(T + C)
Y unit	kPa
Coeff. A	1.33125e+01
Coeff. B	-1.37784e+03
Coeff. C	-2.21750e+01
Reference	Ditter, Perrine, et al., 1961
Comment	Coefficents calculated by NIST from author's data.
Temperature range (K), min.	118.30
Temperature range (K), max.	180.80

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19287457&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Mathews (1972), critical constants of inorganic substances:	https://doi.org/10.1021/cr60275a004
Staveley, Lobo and Calado (1981), triple points:	https://doi.org/10.1016/0011-2275(81)90264-2
Air Liquide Gas Encyclopedia:	http://encyclopedia.airliquide.com/Encyclopedia.asp?GasID=21

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
pc:	Critical Pressure
pvap:	Vapor pressure
rhog:	Gas Density
rhol:	Liquid Density

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature

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