Bromine

Other names:	Br2
	Brom
	Brome
	Bromo
	Broom
	Dibromine
	UN 1744
Inchi:	InChI=1S/Br2/c1-2
InchiKey:	GDTBXPJZTBHREO-UHFFFAOYSA-N
Formula:	Br2
SMILES:	BrBr
Mol. weight [g/mol]:	159.81
CAS:	7726-95-6

Physical Properties

Property code	Value	Unit	Source
ea	2.51 ± 0.10	eV	NIST Webbook
ea	2.87 ± 0.14	eV	NIST Webbook
ea	2.42	eV	NIST Webbook
ea	2.60 ± 0.20	eV	NIST Webbook
ea	2.62 ± 0.20	eV	NIST Webbook
ea	2.55 ± 0.10	eV	NIST Webbook
ea	1.47 ± 0.05	eV	NIST Webbook
gf	-22.24	kJ/mol	Joback Method
hf	30.91 ± 0.11	kJ/mol	NIST Webbook
hfus	6.33	kJ/mol	Joback Method
hvap	28.46	kJ/mol	Joback Method
ie	10.56 ± 0.01	eV	NIST Webbook
ie	10.92	eV	NIST Webbook
ie	10.51	eV	NIST Webbook
ie	10.70 ± 0.10	eV	NIST Webbook
ie	10.52 ± 0.01	eV	NIST Webbook
ie	10.51 ± 0.01	eV	NIST Webbook
ie	10.55	eV	NIST Webbook
ie	10.57	eV	NIST Webbook
ie	10.80 ± 0.20	eV	NIST Webbook
ie	10.52 ± 0.00	eV	NIST Webbook

ie	10.52 ± 0.00	eV	NIST Webbook
ie	10.52 ± 0.01	eV	NIST Webbook
ie	10.51 ± 0.02	eV	NIST Webbook
ie	10.50 ± 0.30	eV	NIST Webbook
ie	10.52 ± 0.01	eV	NIST Webbook
ie	10.51	eV	NIST Webbook
ie	10.52	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.691		Crippen Method
mcvol	45.860	ml/mol	McGowan Method
pc	8573.39	kPa	Joback Method
sgb	245.47 ± 0.01	J/mol×K	NIST Webbook
sl	152.21 ± 0.30	J/mol×K	NIST Webbook
tb	331.72	K	Joback Method
tc	544.73	K	Joback Method
tf	254.15 ± 10.00	K	NIST Webbook
tf	266.00 ± 0.30	K	NIST Webbook
vc	0.160	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	36.78	J/mol×K	509.23	Joback Method
cpg	36.36	J/mol×K	438.23	Joback Method
cpg	35.99	J/mol×K	402.72	Joback Method
cpg	35.50	J/mol×K	367.22	Joback Method
cpg	34.86	J/mol×K	331.72	Joback Method
cpg	36.62	J/mol×K	473.73	Joback Method
cpg	36.86	J/mol×K	544.73	Joback Method
dvisc	0.0024769	Pa×s	209.36	Joback Method
dvisc	0.0005255	Pa×s	331.72	Joback Method
dvisc	0.0006252	Pa×s	311.33	Joback Method
dvisc	0.0007622	Pa×s	290.93	Joback Method
dvisc	0.0009574	Pa×s	270.54	Joback Method
dvisc	0.0012482	Pa×s	250.15	Joback Method
dvisc	0.0017056	Pa×s	229.75	Joback Method
hvapt	17.60	kJ/mol	206.00	NIST Webbook
hvapt	29.80	kJ/mol	363.00	NIST Webbook
hvapt	31.30	kJ/mol	343.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47457e+01
Coeff. B	-3.04378e+03
Coeff. C	-3.13500e+01
Temperature range (K), min.	265.85
Temperature range (K), max.	584.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.30793e+02
Coeff. B	-1.11621e+04
Coeff. C	-3.41575e+01
Coeff. D	5.20176e-05
Temperature range (K), min.	243.15
Temperature range (K), max.	354.00

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Standard molar enthalpies of formation of hydroxy-, chlor-, and bromapatite: https://www.doi.org/10.1016/j.jct.2005.01.010

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7726956&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1948

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
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
pvap:	Vapor pressure
sgb:	Molar entropy at standard conditions (1 bar)
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume