Benzene, 1,2-dibromo-

Other names:	1,2-DIBROMOBENZENE
	Benzene, o-dibromo-
	O-dichlorobenzene
	o-Dibromobenzene
	ortho-Dibromobenzene
Inchi:	InChI=1S/C6H4Br2/c7-5-3-1-2-4-6(5)8/h1-4H
InchiKey:	WQONPSCCEXUXTQ-UHFFFAOYSA-N
Formula:	C6H4Br2
SMILES:	Brc1ccccc1Br
Mol. weight [g/mol]:	235.90
CAS:	583-53-9

Physical Properties

Property code	Value	Unit	Source
gf	131.06	kJ/mol	Joback Method
hf	110.55	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	44.76	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	8.91 ± 0.02	eV	NIST Webbook
ie	8.98 ± 0.02	eV	NIST Webbook
ie	8.99 ± 0.03	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
log10ws	-3.50		Aqueous Solubility Prediction Method
log10ws	-3.50		Estimated Solubility Method
logp	3.212		Crippen Method
mcvol	106.640	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1185.30		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1185.30		NIST Webbook
rinpol	1221.00		NIST Webbook

ripol	1830.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1830.00		NIST Webbook
tb	498.20	K	NIST Webbook
tc	757.23	K	Joback Method
tf	275.00 ± 1.50	K	NIST Webbook
tf	274.95 ± 0.50	K	NIST Webbook
tf	278.42 ± 0.05	K	NIST Webbook
tf	280.00 ± 0.02	K	NIST Webbook
tf	279.52	K	Aqueous Solubility Prediction Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.98	J/mol×K	500.66	Joback Method
cpg	172.09	J/mol×K	543.42	Joback Method
cpg	179.47	J/mol×K	586.18	Joback Method
cpg	186.19	J/mol×K	628.94	Joback Method
cpg	192.30	J/mol×K	671.70	Joback Method
cpg	197.86	J/mol×K	714.47	Joback Method
cpg	202.93	J/mol×K	757.23	Joback Method
cpl	177.44	J/mol×K	283.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.83	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.12	J/mol×K	287.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	178.43	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.75	J/mol×K	291.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.08	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.42	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.76	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.12	J/mol×K	299.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.48	J/mol×K	301.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.85	J/mol×K	303.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.22	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	181.60	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.99	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.38	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.77	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	183.17	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	183.57	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	183.97	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.38	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	184.79	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	190.69	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.60	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.01	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.42	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.82	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	187.23	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	187.63	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	188.03	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	188.42	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	188.82	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	189.20	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	189.58	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	189.96	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	190.33	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.19	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	196.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0018711	Pa×s	315.92	Joback Method
dvisc	0.0012528	Pa×s	346.71	Joback Method
dvisc	0.0008955	Pa×s	377.50	Joback Method
dvisc	0.0006734	Pa×s	408.29	Joback Method
dvisc	0.0004259	Pa×s	469.87	Joback Method
dvisc	0.0003533	Pa×s	500.66	Joback Method
dvisc	0.0005270	Pa×s	439.08	Joback Method
hfust	12.61	kJ/mol	275.00	NIST Webbook

hfust	12.61	kJ/mol	275.00	NIST Webbook
hfust	13.59	kJ/mol	274.95	NIST Webbook
hvapt	50.10	kJ/mol	478.00	NIST Webbook
sfust	49.40	J/mol×K	274.95	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37724e+01
Coeff. B	-3.84834e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	365.02
Temperature range (K), max.	534.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.83542e+01
Coeff. B	-9.17476e+03
Coeff. C	-9.05766e+00
Coeff. D	3.73877e-06
Temperature range (K), min.	388.15
Temperature range (K), max.	568.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=1674
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1674.mol
Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:	https://www.doi.org/10.1021/je600573w
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583539&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume