Benzene, 1,3-dibromo-

Other names:	1,3-DIBROMOBENZENE
	Benzene, m-dibromo-
	m-Dibromobenzene
Inchi:	InChI=1S/C6H4Br2/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	JSRLURSZEMLAFO-UHFFFAOYSA-N
Formula:	C6H4Br2
SMILES:	Brc1cccc(Br)c1
Mol. weight [g/mol]:	235.90
CAS:	108-36-1

Physical Properties

Property code	Value	Unit	Source
gf	131.06	kJ/mol	Joback Method
hf	110.55	kJ/mol	Joback Method
hfpi	1000.00 ± 10.00	kJ/mol	NIST Webbook
hfpiz	1020.00 ± 10.00	kJ/mol	NIST Webbook
hfus	15.52	kJ/mol	Joback Method
hvap	44.76	kJ/mol	Joback Method
ie	9.01 ± 0.02	eV	NIST Webbook
ie	8.95 ± 0.02	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	9.05 ± 0.03	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	9.01 ± 0.05	eV	NIST Webbook
log10ws	-3.54		Aqueous Solubility Prediction Method
log10ws	-3.54		Estimated Solubility Method
logp	3.212		Crippen Method
mcvol	106.640	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1162.20		NIST Webbook
rinpol	1190.00		NIST Webbook

rinpol	1162.20		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1756.00		NIST Webbook
tb	491.20	K	NIST Webbook
tc	757.23	K	Joback Method
tf	266.25 ± 0.50	K	NIST Webbook
tf	266.00 ± 1.50	K	NIST Webbook
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.93	J/mol×K	757.23	Joback Method
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
cpl	178.08	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.01	J/mol×K	283.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.40	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.71	J/mol×K	287.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	177.04	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.38	J/mol×K	291.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.72	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	189.09	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.44	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.81	J/mol×K	299.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.19	J/mol×K	301.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.58	J/mol×K	303.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.97	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	180.37	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.78	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.19	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.60	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.01	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.43	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.85	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	183.28	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	189.47	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.13	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.55	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.98	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.40	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.83	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.25	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.67	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	187.08	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	187.49	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	187.90	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	188.30	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	188.70	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	192.00	J/mol×K	298.15	NIST Webbook
cpl	183.70	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	189.85	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0004259	Pa×s	469.87	Joback Method
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	0.0005270	Pa×s	439.08	Joback Method
dvisc	0.0003533	Pa×s	500.66	Joback Method
dvisc	0.0006734	Pa×s	408.29	Joback Method
hfust	14.22	kJ/mol	266.25	NIST Webbook
hfust	13.21	kJ/mol	266.30	NIST Webbook
hfust	13.21	kJ/mol	266.30	NIST Webbook
hvapt	48.30	kJ/mol	458.50	NIST Webbook
sfust	53.40	J/mol×K	266.25	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.20	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43239e+01
Coeff. B	-4.02376e+03
Coeff. C	-7.66160e+01
Temperature range (K), min.	363.28
Temperature range (K), max.	523.09

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.02731e+01
Coeff. B	-9.55542e+03
Coeff. C	-1.08844e+01
Coeff. D	5.13030e-06
Temperature range (K), min.	266.25
Temperature range (K), max.	761.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1675.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:	https://www.doi.org/10.1021/je600573w
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108361&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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=1675
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume