

# Benzene, 1,2-dibromo-

<b>Other names:</b>	1,2-DIBROMOBENZENE Benzene, o-dibromo- O-dichlorobenzene o-Dibromobenzene ortho-Dibromobenzene
<b>Inchi:</b>	InChI=1S/C6H4Br2/c7-5-3-1-2-4-6(5)8/h1-4H
<b>InchiKey:</b>	WQONPSCCEXUXTQ-UHFFFAOYSA-N
<b>Formula:</b>	C6H4Br2
<b>SMILES:</b>	BrC1ccccc1Br
<b>Mol. weight [g/mol]:</b>	235.90
<b>CAS:</b>	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	8.91 ± 0.02	eV	NIST Webbook
ie	8.98 ± 0.02	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	8.99 ± 0.03	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-3.50		Estimated Solubility Method
log10ws	-3.50		Aqueous Solubility Prediction Method
logp	3.212		Crippen Method
mcvol	106.640	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
rinpol	1185.30		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1185.30		NIST Webbook
rinpol	1221.00		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	280.00 ± 0.02	K	NIST Webbook
tf	274.95 ± 0.50	K	NIST Webbook
tf	275.00 ± 1.50	K	NIST Webbook
tf	278.42 ± 0.05	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	202.93	J/mol×K	757.23	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	163.98	J/mol×K	500.66	Joback Method
cpg	172.09	J/mol×K	543.42	Joback Method
cpl	179.08	J/mol×K	293.15	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 Bzenes
cpl	181.22	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	181.60	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	181.99	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	182.38	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	182.77	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	183.17	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	183.57	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	183.97	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes

cpl	184.38	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	184.79	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	185.19	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	185.60	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	186.01	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	186.42	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	186.82	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	187.23	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes

cpl	187.63	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	179.76	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	188.42	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	188.82	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	189.20	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	189.58	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	189.96	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	190.33	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	190.69	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes

cpl	179.42	J/mol×K	295.15	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	178.43	J/mol×K	289.15	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	177.83	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	196.80	J/mol×K	298.15	NIST Webbook
cpl	177.44	J/mol×K	283.15	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
dvisc	0.0006734	Paxs	408.29	Joback Method
dvisc	0.0008955	Paxs	377.50	Joback Method
dvisc	0.0012528	Paxs	346.71	Joback Method
dvisc	0.0003533	Paxs	500.66	Joback Method
dvisc	0.0004259	Paxs	469.87	Joback Method
dvisc	0.0018711	Paxs	315.92	Joback Method
dvisc	0.0005270	Paxs	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	$\ln(P_{\text{vp}}) = A + B/(T + C)$
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	$\ln(P_{\text{vp}}) = A + B/T + C*\ln(T) + D*T^2$
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

<b>KDB:</b>	<a href="https://www.cheric.org/files/research/kdb/mol/mol1674.mol">https://www.cheric.org/files/research/kdb/mol/mol1674.mol</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xi20040112_053635.txt</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C583539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C583539&amp;Units=SI</a>
<b>Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Iodo-Yaws Handbook of Vapor-Pressures:</b>	<a href="https://www.doi.org/10.1021/je600573w">https://www.doi.org/10.1021/je600573w</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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