

Benzene, 1-bromo-2-chloro-

Other names:	1-Bromo-2-chlorobenzene 1-Chloro-2-bromobenzene 2-Bromo-1-chlorobenzene 2-Bromochlorobenzene 2-Chlorobromobenzene o-Bromochlorobenzene o-Chlorobromobenzene
Inchi:	InChI=1S/C6H4BrCl/c7-5-3-1-2-4-6(5)8/h1-4H
InchiKey:	QBELEDRHMPMKHP-UHFFFAOYSA-N
Formula:	C6H4BrCl
SMILES:	Clc1ccccc1Br
Mol. weight [g/mol]:	191.45
CAS:	694-80-4

Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	68.48	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	42.71	kJ/mol	Joback Method
log10ws	-3.19		Estimated Solubility Method
log10ws	-3.19		Aqueous Solubility Prediction Method
logp	3.103		Crippen Method
mcvol	101.380	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
rinpol	188.00		NIST Webbook
rinpol	1137.48		NIST Webbook
rinpol	1111.54		NIST Webbook
rinpol	1123.72		NIST Webbook
rinpol	1097.60		NIST Webbook
rinpol	1097.60		NIST Webbook
rinpol	1105.74		NIST Webbook
rinpol	1110.94		NIST Webbook
rinpol	1116.38		NIST Webbook
rinpol	1097.60		NIST Webbook

rinpol	1111.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	188.00		NIST Webbook
rinpol	1137.48		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1120.00		NIST Webbook
ripol	1633.76		NIST Webbook
ripol	1650.41		NIST Webbook
ripol	1665.31		NIST Webbook
ripol	1653.05		NIST Webbook
tb	477.20	K	NIST Webbook
tb	468.00	K	NIST Webbook
tc	716.18	K	Joback Method
tf	260.50	K	Aqueous Solubility Prediction Method
tf	261.00	K	NIST Webbook
tf	260.55 ± 0.20	K	NIST Webbook
vc	0.374	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.69	J/mol×K	471.93	Joback Method
cpg	197.22	J/mol×K	716.18	Joback Method
cpg	191.83	J/mol×K	675.47	Joback Method
cpg	185.95	J/mol×K	634.76	Joback Method
cpg	179.54	J/mol×K	594.05	Joback Method
cpg	164.95	J/mol×K	512.64	Joback Method
cpg	172.55	J/mol×K	553.35	Joback Method
cpl	176.90	J/mol×K	298.15	NIST Webbook
cpl	184.05	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	183.62	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	184.47	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.89	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	183.20	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.31	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.72	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.13	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	186.53	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	172.25	J/mol×K	283.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	172.59	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	172.94	J/mol×K	287.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	173.29	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	173.65	J/mol×K	291.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.02	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.39	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.78	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	175.17	J/mol×K	299.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	175.56	J/mol×K	301.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	182.33	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.36	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.77	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.19	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.61	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.03	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.45	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.88	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	179.31	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	179.74	J/molxK	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.17	J/molxK	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	180.60	J/molxK	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.03	J/molxK	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.47	J/molxK	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.90	J/molxK	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	175.96	J/molxK	303.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	182.77	J/molxK	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0020482	Paxs	286.04	Joback Method
dvisc	0.0009042	Paxs	348.00	Joback Method
dvisc	0.0013076	Paxs	317.02	Joback Method
dvisc	0.0003355	Paxs	471.93	Joback Method

dvisc	0.0004080	Paxs	440.95	Joback Method
dvisc	0.0005111	Paxs	409.97	Joback Method
dvisc	0.0006641	Paxs	378.99	Joback Method
hfust	12.37	kJ/mol	260.55	NIST Webbook
hfust	12.37	kJ/mol	260.60	NIST Webbook
sfust	47.50	J/mol×K	260.55	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Iodo-substituted Benzenes:	https://www.doi.org/10.1021/je600573w
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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

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