

Benzene, 1-bromo-3-chloro-

Other names:	1-Bromo-3-chlorobenzene 1-Chloro-3-bromobenzene 3-Bromo-1-chlorobenzene 3-Bromochlorobenzene 3-Chlorobromobenzene 3-Chlorophenyl bromide NSC 53548 m-Bromochlorobenzene m-Bromophenyl chloride m-Chlorobromobenzene m-Chlorophenyl bromide
Inchi:	InChI=1S/C6H4BrCl/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	JRGGUPZKKTVKOV-UHFFFAOYSA-N
Formula:	C6H4BrCl
SMILES:	Clc1cccc(Br)c1
Mol. weight [g/mol]:	191.45
CAS:	108-37-2

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	-3.21		Estimated Solubility Method
log10ws	-3.21		Aqueous Solubility Prediction Method
logp	3.103		Crippen Method
mcvol	101.380	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
tb	469.00 ± 0.07	K	NIST Webbook
tb	469.20	K	NIST Webbook
tb	469.00	K	NIST Webbook
tc	716.18	K	Joback Method

tf	251.40	K	Aqueous Solubility Prediction Method
tf	252.00	K	NIST Webbook
tf	251.67 ± 0.05	K	NIST Webbook
tf	252.00 ± 2.00	K	NIST Webbook
tf	251.95 ± 0.50	K	NIST Webbook
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.22	J/mol×K	716.18	Joback Method
cpg	172.55	J/mol×K	553.35	Joback Method
cpg	179.54	J/mol×K	594.05	Joback Method
cpg	185.95	J/mol×K	634.76	Joback Method
cpg	191.83	J/mol×K	675.47	Joback Method
cpg	156.69	J/mol×K	471.93	Joback Method
cpg	164.95	J/mol×K	512.64	Joback Method
cpl	172.97	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.15	J/mol×K	299.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.56	J/mol×K	301.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	174.98	J/mol×K	303.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	175.40	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	175.82	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	176.25	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	176.68	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	177.12	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	177.56	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	178.00	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	178.44	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	178.89	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes

cpl	179.33	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	179.78	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	180.23	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	180.68	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	181.13	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	181.58	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	182.03	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	173.75	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes

cpl	182.92	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	183.36	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	183.80	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	184.24	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	184.67	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	185.10	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	185.52	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	185.94	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes
cpl	173.36	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Bzenes

cpl	172.59	J/mol×K	291.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	172.21	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	171.84	J/mol×K	287.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	171.49	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.90	J/mol×K	298.15	NIST Webbook
cpl	182.47	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	171.14	J/mol×K	283.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0006641	Paxs	378.99	Joback Method
dvisc	0.0009042	Paxs	348.00	Joback Method
dvisc	0.0013076	Paxs	317.02	Joback Method
dvisc	0.0020482	Paxs	286.04	Joback Method
dvisc	0.0004080	Paxs	440.95	Joback Method
dvisc	0.0005111	Paxs	409.97	Joback Method
dvisc	0.0003355	Paxs	471.93	Joback Method
hfust	12.29	kJ/mol	252.00	NIST Webbook
hfust	12.29	kJ/mol	251.95	NIST Webbook
hvapt	52.20	kJ/mol	360.50	NIST Webbook
sfust	48.80	J/mol×K	251.95	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49420e+01
Coeff. B	-4.39672e+03
Coeff. C	-4.32640e+01
Temperature range (K), min.	308.00
Temperature range (K), max.	499.80

Sources

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/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108372&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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
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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