

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
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		Aqueous Solubility Prediction Method
log10ws	-3.21		Estimated Solubility 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	K	NIST Webbook
tb	469.00 ± 0.07	K	NIST Webbook
tb	469.20	K	NIST Webbook
tc	716.18	K	Joback Method

tf	251.95 ± 0.50	K	NIST Webbook
tf	252.00 ± 2.00	K	NIST Webbook
tf	251.67 ± 0.05	K	NIST Webbook
tf	252.00	K	NIST Webbook
tf	251.40	K	Aqueous Solubility Prediction Method
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	156.69	J/mol×K	471.93	Joback Method
cpg	164.95	J/mol×K	512.64	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
cpl	172.59	J/mol×K	291.15	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
cpl	171.49	J/mol×K	285.15	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	172.21	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	185.52	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	172.97	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	173.36	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	173.75	J/mol×K	297.15	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 Benzenes	

cpl	175.82	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.25	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	176.68	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.12	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	177.56	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.00	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.44	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	181.90	J/mol×K	298.15	NIST Webbook
cpl	179.33	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	179.78	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	180.23	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	180.68	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	181.13	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	181.58	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	182.03	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	182.47	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	182.92	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	
cpl	183.36	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes	

cpl	183.80	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.24	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	184.67	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.10	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	178.89	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	185.94	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
dvisc	0.0004080	Pa×s	440.95	Joback Method
dvisc	0.0020482	Pa×s	286.04	Joback Method
dvisc	0.0013076	Pa×s	317.02	Joback Method
dvisc	0.0009042	Pa×s	348.00	Joback Method
dvisc	0.0006641	Pa×s	378.99	Joback Method
dvisc	0.0005111	Pa×s	409.97	Joback Method
dvisc	0.0003355	Pa×s	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

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/ci990307l
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/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
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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