Benzene, bromo-

Other names:	1-Bromobenzene
	Bromobenzene
	MONOBROMOBENZENE
	NCI-C55492
	PHENYL BROMIDE
	UN 2514
Inchi:	InChI=1S/C6H5Br/c7-6-4-2-1-3-5-6/h1-5H
InchiKey:	QARVLSVVCXYDNA-UHFFFAOYSA-N
Formula:	C6H5Br
SMILES:	Brc1ccccc1
Mol. weight [g/mol]:	157.01
CAS:	108-86-1

Physical Properties

Property code	Value	Unit	Source
af	0.2510		KDB
affp	754.10	kJ/mol	NIST Webbook
aigt	838.15	K	KDB
basg	725.80	kJ/mol	NIST Webbook
chl	-3111.90 ± 0.67	kJ/mol	NIST Webbook
dm	1.50	debye	KDB
fpo	324.26	K	KDB
gf	138.60	kJ/mol	KDB
hf	105.10	kJ/mol	KDB
hfl	60.90 ± 4.10	kJ/mol	NIST Webbook
hfl	58.60	kJ/mol	NIST Webbook
hfus	10.62	kJ/mol	Joback Method
hvap	44.50 ± 0.10	kJ/mol	NIST Webbook
hvap	44.54 ± 0.04	kJ/mol	NIST Webbook
hvap	44.80	kJ/mol	NIST Webbook
hvap	44.54	kJ/mol	NIST Webbook
hvap	37.90 ± 0.03	kJ/mol	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	8.98 ± 0.02	eV	NIST Webbook
ie	9.05 ± 0.02	eV	NIST Webbook
ie	9.02	eV	NIST Webbook

ie	8.99	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.00 ± 0.03	eV	NIST Webbook
ie	8.97 ± 0.02	eV	NIST Webbook
ie	9.03 ± 0.01	eV	NIST Webbook
ie	8.98 ± 0.03	eV	NIST Webbook
ie	8.95	eV	NIST Webbook
ie	8.98 ± 0.02	eV	NIST Webbook
ie	8.99	eV	NIST Webbook
ie	8.99 ± 0.03	eV	NIST Webbook
ie	9.04	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.55		Aqueous Solubility Prediction Method
log10ws	-2.55		Estimated Solubility Method
logp	2.449		Crippen Method
mcvol	89.140	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4520.00	kPa	KDB
rinpol	926.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	150.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	926.64		NIST Webbook
rinpol	921.35		NIST Webbook
rinpol	919.67		NIST Webbook
rinpol	909.50		NIST Webbook
rinpol	903.90		NIST Webbook

rinpol	941.00		NIST Webbook
rinpol	979.60		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	959.60		NIST Webbook
rinpol	934.80		NIST Webbook
rinpol	923.70		NIST Webbook
rinpol	914.70		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	941.36		NIST Webbook
rinpol	931.71		NIST Webbook
rinpol	952.20		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	925.80		NIST Webbook
ripol	1381.03		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1391.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1348.92		NIST Webbook
ripol	1358.59		NIST Webbook
ripol	1373.68		NIST Webbook
sl	207.90	J/mol×K	NIST Webbook
sl	21922.00	J/mol×K	NIST Webbook
tb	429.21	K	KDB
tc	670.00	K	KDB
tf	242.50	K	KDB
tf	242.25	K	Aqueous Solubility Prediction Method
tt	242.42 ± 0.02	K	NIST Webbook
tt	242.40	K	KDB
tt	242.40 ± 0.01	K	NIST Webbook
tt	242.40 ± 0.20	K	NIST Webbook
vc	0.324	m3/kmol	KDB
zc	0.2628890		KDB

zra	0.26	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.06	J/mol×K	626.10	Joback Method
cpg	144.94	J/mol×K	468.84	Joback Method
cpg	153.71	J/mol×K	508.15	Joback Method
cpg	161.79	J/mol×K	547.47	Joback Method
cpg	169.22	J/mol×K	586.78	Joback Method
cpg	182.34	J/mol×K	665.41	Joback Method
cpg	135.44	J/mol×K	429.52	Joback Method
cpl	151.50	J/mol×K	293.20	NIST Webbook
cpl	145.60	J/mol×K	302.60	NIST Webbook
cpl	127.60	J/mol×K	231.70	NIST Webbook
cpl	155.39	J/mol×K	298.10	NIST Webbook
cpl	145.60	J/mol×K	302.60	NIST Webbook
cpl	153.54	J/mol×K	293.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	155.90	J/mol×K	303.15	NIST Webbook
cpl	167.15	J/mol×K	353.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	166.69	J/mol×K	351.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	166.23	J/mol×K	349.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	165.76	J/mol×K	347.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	165.30	J/mol×K	345.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	164.83	J/mol×K	343.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	164.36	J/mol×K	341.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	163.89	J/mol×K	339.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	163.42	J/mol×K	337.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	162.95	J/mol×K	335.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	162.00	J/mol×K	331.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	161.53	J/mol×K	329.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	161.06	J/mol×K	327.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	160.60	J/mol×K	325.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	151.00	J/mol×K	298.00	NIST Webbook
cpl	160.13	J/mol×K	323.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	159.66	J/mol×K	321.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	159.20	J/mol×K	319.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	158.74	J/mol×K	317.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	158.28	J/mol×K	315.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	157.83	J/mol×K	313.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	157.38	J/mol×K	311.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	152.37	J/mol×K	287.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	156.49	J/mol×K	307.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	162.48	J/mol×K	333.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	155.62	J/mol×K	303.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	155.19	J/mol×K	301.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	154.77	J/mol×K	299.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	156.05	J/mol×K	305.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	154.35	J/mol×K	297.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

cpl	153.94	J/mol×K	295.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	151.63	J/mol×K	283.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	151.99	J/mol×K	285.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	156.93	J/mol×K	309.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	152.75	J/mol×K	289.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	153.14	J/mol×K	291.15	Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes
cpl	154.29	J/mol×K	298.15	NIST Webbook
dvisc	0.0011640	Pa×s	293.00	Thermophysical Properties of Binary Mixtures of Methanol with Chlorobenzene and Bromobenzene from 293K to 313K

dvisc	0.0009640	Pa×s	308.15	Thermophysical Properties For Diethylene Glycol + Nitrobenzene and Triethylene Glycol + (Chloro-, Bromo-, Nitro-) Benzene Systems at Different Temperatures
dvisc	0.0010410	Pa×s	298.15	Thermophysical Properties For Diethylene Glycol + Nitrobenzene and Triethylene Glycol + (Chloro-, Bromo-, Nitro-) Benzene Systems at Different Temperatures
dvisc	0.0008780	Pa×s	313.15	Thermophysical properties of the binary mixtures of 1,2-Dichloroethane with Chlorobenzene and Bromobenzene from 298.15 to 313.15 K
dvisc	0.0009540	Pa×s	308.15	Thermophysical properties of the binary mixtures of 1,2-Dichloroethane with Chlorobenzene and Bromobenzene from 298.15 to 313.15 K
dvisc	0.0010146	Pa×s	303.15	Thermophysical properties of the binary mixtures of 1,2-Dichloroethane with Chlorobenzene and Bromobenzene from 298.15 to 313.15 K

dvisc	0.0010820	Pa×s	298.15	Thermophysical properties of the binary mixtures of 1,2-Dichloroethane with Chlorobenzene and Bromobenzene from 298.15 to 313.15 K
dvisc	0.0008786	Pa×s	313.00	Thermophysical Properties of Binary Mixtures of Methanol with Chlorobenzene and Bromobenzene from 293K to 313K
dvisc	0.0009844	Pa×s	303.00	Thermophysical Properties of Binary Mixtures of Methanol with Chlorobenzene and Bromobenzene from 293K to 313K
hfust	10.70	kJ/mol	242.40	NIST Webbook
hfust	10.63	kJ/mol	242.43	NIST Webbook
hfust	10.70	kJ/mol	242.40	NIST Webbook
hfust	10.70	kJ/mol	242.40	NIST Webbook
hvapt	42.50	kJ/mol	429.10	KDB
hvapt	42.30	kJ/mol	398.00	NIST Webbook
hvapt	42.40	kJ/mol	378.00	NIST Webbook
hvapt	44.00	kJ/mol	293.00	NIST Webbook
pvap	0.38	kPa	292.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.35	kPa	291.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.44	kPa	294.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.32	kPa	289.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.52	kPa	297.40	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.25	kPa	286.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.25	kPa	285.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.21	kPa	283.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.20	kPa	282.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.64	kPa	300.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.13	kPa	276.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	95.30	kPa	426.85	Vapor-liquid equilibrium for the binary mixtures of dimethylsulfoxide with substituted benzenes
pvap	0.46	kPa	295.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.76	kPa	303.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.40	kPa	293.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.15	kPa	278.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.30	kPa	288.30	Thermochemistry of Halogen-Substituted Methylbenzenes

rfi	1.55340	308.15	Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K
rfi	1.55610	303.15	Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K
rfi	1.55710	298.15	Activity coefficients and excess Gibbs energy of binary mixtures of N,N-dimethyl formamide with selected compounds at 95.5 kPa
rfi	1.54970	313.15	Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K
rfi	1.55710	298.15	(Vapor + liquid) equilibrium of the binary mixtures formed by acetonitrile with selected compounds at 95.5 kPa

rfi	1.55420	303.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K
rfi	1.55140	308.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K
rfi	1.55770	298.15	Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K
rfi	1.55710	293.15	Excess Gibbs energies of binary mixtures formed by nitrobenzene with selected compounds at 94.95 kPa

rfi	1.55460		303.15	Excess Volumes of Binary Solutions of Methyl Formate, Ethyl Formate, Propyl Formate, and Benzyl Acetate with Bromo-, Chloro-, and Nitrobenzenes at (303.15, 308.15, and 313.15) K
rhol	1481.97	kg/m3	303.15	Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K
rhol	1468.41	kg/m3	313.15	Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K
rhol	1454.85	kg/m3	323.15	Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K
rhol	1495.52	kg/m3	293.15	Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K

rhol	1481.52	kg/m3	303.15	Studies on the importance of nature of substituent on the thermodynamic and transport properties of liquid mixtures at various temperatures
rhol	1475.36	kg/m3	308.15	Studies on the importance of nature of substituent on the thermodynamic and transport properties of liquid mixtures at various temperatures
rhol	1468.02	kg/m3	313.15	Studies on the importance of nature of substituent on the thermodynamic and transport properties of liquid mixtures at various temperatures
rhol	1461.36	kg/m3	318.15	Studies on the importance of nature of substituent on the thermodynamic and transport properties of liquid mixtures at various temperatures
rhol	1495.23	kg/m3	293.20	Isobaric Vapor-Liquid Equilibria for Binary Mixtures of 1,2-Dibromoethane with Benzene, Toluene, Fluorobenzene, and Bromobenzene at Atmospheric Pressure

rhol	1495.28	kg/m3	293.20	Isobaric vapour liquid equilibria for binary mixtures of n-heptane with bromobenzene, chlorobenzene and fluorobenzene at atmospheric pressure
rhol	1474.58	kg/m3	308.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Ethyl-1-hexanol with Benzene and Halobenzenes
rhol	1481.40	kg/m3	303.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Ethyl-1-hexanol with Benzene and Halobenzenes
rhol	1488.12	kg/m3	298.15	Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of 2-Ethyl-1-hexanol with Benzene and Halobenzenes
rhol	1495.00	kg/m3	293.00	KDB
rhol	1441.22	kg/m3	333.15	Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K
sfust	43.84	J/mol×K	242.43	NIST Webbook
sfust	44.15	J/mol×K	242.40	NIST Webbook
srf	0.04	N/m	293.20	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	427.85	K	95.30	Excess enthalpies of dimethylsulfoxide with substituted benzenes at 298.15K
tbrp	300.90	K	0.70	NIST Webbook
tfp	374.75	K	900000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	310.05	K	400000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	322.55	K	500000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	336.15	K	600000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa

tfp	349.25	K	700000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	361.85	K	800000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	292.45	K	300000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	382.85	K	1000000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa
tfp	430.05	K	1500000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa

tfp	473.67	K	2000000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa	
tfp	514.22	K	2500000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa	
tfp	553.94	K	3000000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa	
tfp	587.21	K	3500000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa	
tfp	276.45	K	200000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa	

tfp	259.05	K	100000.00	Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44191e+01
Coeff. B	-3.72354e+03
Coeff. C	-4.91780e+01
Temperature range (K), min.	312.67
Temperature range (K), max.	458.01

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.92440e+01
Coeff. B	-7.92948e+03
Coeff. C	-9.41640e+00
Coeff. D	5.04459e-06
Temperature range (K), min.	242.43
Temperature range (K), max.	670.15

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid

248.15	99.70	1554.489
248.15	1231.41	1555.368
248.15	2075.45	1556.036
248.15	4196.22	1557.697
248.15	5950.98	1559.054
248.15	8068.32	1560.666
248.15	10015.40	1562.113
248.15	11951.60	1563.577
248.15	13994.80	1565.093
248.15	15940.30	1566.527
248.15	18145.00	1568.122
248.15	19946.50	1569.417
248.15	21965.00	1570.861
248.15	24135.90	1572.41
248.15	25864.70	1573.623
248.15	27917.30	1575.05
248.15	29850.30	1576.387
273.15	100.51	1520.557
273.15	1116.26	1521.447
273.15	2128.10	1522.34
273.15	4045.82	1524.026
273.15	5967.30	1525.66
273.15	8142.83	1527.515
273.15	10020.30	1529.109
273.15	11896.10	1530.677
273.15	13922.00	1532.353
273.15	16083.00	1534.134
273.15	18195.20	1535.834
273.15	20035.10	1537.31
273.15	21829.30	1538.747
273.15	23856.50	1540.342
273.15	25976.20	1542.017
273.15	28097.70	1543.651
273.15	29947.00	1545.093
293.15	101.93	1493.557
293.15	1239.69	1494.684
293.15	2010.73	1495.408
293.15	4059.70	1497.371
293.15	6007.85	1499.218
293.15	8079.77	1501.16
293.15	10000.80	1502.944
293.15	11960.00	1504.732
293.15	14168.60	1506.732
293.15	15878.80	1508.265

293.15	17960.30	1510.109
293.15	19999.40	1511.901
293.15	21880.00	1513.531
293.15	24122.20	1515.458
293.15	26141.00	1517.174
293.15	28060.50	1518.79
293.15	29992.70	1520.418
313.15	102.54	1466.553
313.15	2000.76	1468.587
313.15	4010.97	1470.712
313.15	6189.56	1473.0
313.15	7991.64	1474.858
313.15	10089.40	1477.007
313.15	12142.80	1479.063
313.15	14014.60	1480.929
313.15	16087.30	1482.944
313.15	18046.60	1484.852
313.15	20004.20	1486.73
313.15	22154.30	1488.763
313.15	23944.20	1490.446
313.15	26099.80	1492.424
313.15	28042.50	1494.215
313.15	29905.50	1495.902
333.15	100.42	1439.385
333.15	1115.03	1440.596
333.15	1943.37	1441.571
333.15	4094.54	1444.097
333.15	6114.22	1446.439
333.15	7927.80	1448.512
333.15	10021.70	1450.842
333.15	11958.50	1453.001
333.15	13999.00	1455.239
333.15	16048.70	1457.443
333.15	18155.70	1459.682
333.15	20007.80	1461.631
333.15	22157.50	1463.842
333.15	24129.60	1465.857
333.15	26094.50	1467.846
333.15	28018.50	1469.764
333.15	29890.30	1471.607
353.15	99.80	1411.936
353.15	1173.75	1413.368
353.15	1944.34	1414.39
353.15	3949.81	1417.013

353.15	5968.93	1419.612
353.15	7990.46	1422.164
353.15	9916.05	1424.555
353.15	11986.60	1427.088
353.15	14134.60	1429.674
353.15	15921.30	1431.797
353.15	18146.30	1434.386
353.15	19873.50	1436.374
353.15	22180.00	1438.986
353.15	23963.50	1440.977
353.15	26085.20	1443.316
353.15	28122.10	1445.529
353.15	29956.10	1447.501
373.15	98.54	1384.068
373.15	1150.11	1385.641
373.15	2174.39	1387.16
373.15	3917.65	1389.708
373.15	6182.40	1392.956
373.15	8042.69	1395.57
373.15	10003.40	1398.276
373.15	12007.70	1400.991
373.15	14086.40	1403.757
373.15	15912.60	1406.155
373.15	18065.60	1408.912
373.15	19882.10	1411.213
373.15	22174.10	1414.047
373.15	24052.60	1416.329
373.15	25897.20	1418.541
373.15	27711.00	1420.705
373.15	29530.80	1422.851
393.15	97.33	1355.66
393.15	1226.04	1357.559
393.15	2181.20	1359.152
393.15	3965.26	1362.078
393.15	6075.43	1365.466
393.15	8146.91	1368.751
393.15	9937.30	1371.465
393.15	11969.70	1374.529
393.15	14177.00	1377.777
393.15	15955.80	1380.344
393.15	18163.70	1383.473
393.15	20146.90	1386.231
393.15	22175.70	1388.998
393.15	23981.50	1391.424

393.15	26169.90	1394.302
393.15	28005.40	1396.697
393.15	29541.50	1398.685
413.15	99.45	1326.547
413.15	1202.85	1328.655
413.15	2177.13	1330.512
413.15	3915.54	1333.735
413.15	6185.52	1337.833
413.15	8176.14	1341.325
413.15	10032.40	1344.48
413.15	12103.60	1348.01
413.15	13991.80	1351.03
413.15	15890.50	1354.115
413.15	18162.20	1357.681
413.15	19933.00	1360.414
413.15	22150.20	1363.736
413.15	24133.10	1366.656
413.15	26038.90	1369.413
413.15	27898.50	1372.058
413.15	29858.00	1374.805
433.15	1243.75	1299.092
433.15	1973.28	1300.66
433.15	4075.91	1305.09
433.15	6197.75	1309.427
433.15	7981.47	1312.955
433.15	10019.80	1316.907
433.15	12072.60	1320.75
433.15	14033.50	1324.335
433.15	15960.20	1327.765
433.15	17921.10	1331.186
433.15	19992.20	1334.752
433.15	21950.20	1337.95
433.15	24017.90	1341.307
433.15	26143.40	1344.678
433.15	28052.40	1347.64
433.15	29864.50	1350.426
453.15	1135.36	1268.141
453.15	1982.45	1270.245
453.15	4017.67	1275.165
453.15	6189.02	1280.221
453.15	7994.19	1284.28
453.15	10138.80	1288.978
453.15	12157.20	1293.201
453.15	13981.80	1296.937

453.15	16133.80	1301.214
453.15	18121.60	1305.054
453.15	19974.20	1308.564
453.15	22140.80	1312.522
453.15	24115.40	1316.051
453.15	26121.30	1319.557
453.15	28034.20	1322.825
453.15	29912.10	1325.979
473.15	1191.19	1236.278
473.15	2175.44	1239.118
473.15	4131.48	1244.576
473.15	5988.10	1249.543
473.15	8161.41	1255.135
473.15	10165.40	1260.077
473.15	12165.90	1264.845
473.15	14162.70	1269.434
473.15	16124.70	1273.802
473.15	18166.70	1278.202
473.15	20146.20	1282.345
473.15	22123.10	1286.362
473.15	24157.00	1290.388
473.15	26074.70	1294.08
473.15	28019.90	1297.733
473.15	29860.30	1301.116

Reference *https://www.doi.org/10.1016/j.jct.2008.02.020*

Sources

Fusion Curves and Enthalpy and Internal Energy Changes of Benzene, Nitrobenzene, Bromobenzene, and Chlorobenzene at Pressures up to 3500 MPa:	https://www.doi.org/10.1021/je700276z
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108861&Units=SI
Isobaric Vapor-Liquid Equilibria for Binary Mixtures of 1,2-Dibromoethane with Benzene, Toluene, Fluorobenzene, and Bromobenzene at Atmospheric Pressure:	https://www.doi.org/10.1021/je050231r
Thermophysical Properties of Binary Mixtures of Methanol with Isobaric vapor-liquid equilibria for binary mixtures of n-heptane with bromobenzene, chlorobenzene and fluorobenzene at atmospheric pressure:	https://www.doi.org/10.1007/s10765-008-0444-7
	https://www.doi.org/10.1016/j.fluid.2005.11.020
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1683.mol
Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes:	https://www.doi.org/10.1021/je600573w
Refractive properties, speed of sound and FT-IR study of binary mixtures of N-formylmorpholine with some halobenzenes at 303.15, 308.15 and 313.15 K:	https://www.doi.org/10.1016/j.fluid.2014.12.012
Densities, Viscosities, Speeds of Sound, and Refractive Indices of Binary Mixtures of Bromobenzene or 2-Ethyl-1-hexanol with Halobenzene Solvents:	https://www.doi.org/10.1007/s10765-013-1526-8
Solubility of Hydrofluorocarbons in Halobenzene Solvents:	https://www.doi.org/10.1021/je500525q
Excess Gibbs energies of binary mixtures formed by nitrobenzene with selected compounds at 94.98 kPa:	https://www.doi.org/10.1016/j.fluid.2006.12.010
Phase behavior of ionic liquids: 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imides with halogenated benzenes:	https://www.doi.org/10.1016/j.jct.2015.04.012

Thermochemistry of Halogen-Substituted Methylbenzenes:	https://www.doi.org/10.1021/je500784s
Volumetric and electromagnetic properties of binary mixtures consist of benzene derivatives at different temperature and ternary mixtures with 1,2-dichloroethane at T = 293.15 K with application of the Prigogine-Flory-Patterson theory and PC-SAFT:	https://www.doi.org/10.1016/j.tca.2016.06.023
Vapor-liquid equilibrium for the binary mixtures of dimethylsulfoxide with substituted benzenes	https://www.doi.org/10.1016/j.fluid.2007.08.001
Solubilities of p-Tolylboronic Acid, Bromobenzene and 4-Phenyltoluene in Carbon Dioxide at Elevated Pressures:	https://www.doi.org/10.1021/je034051y
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Excess enthalpies of dimethylsulfoxide with substituted benzenes at 298.15K:	https://www.doi.org/10.1016/j.fluid.2007.10.017
(Vapor + liquid) equilibrium of the binary mixtures formed by acetonitrile with selected compounds at 95.5 kPa:	https://www.doi.org/10.1016/j.jct.2007.03.007
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Measuring the Aqueous Henry's Law Constant at Elevated Temperatures Using an Extended EPICS Technique:	https://www.doi.org/10.1021/je100701w
Density, Viscosity, Refractive Index, and Speed of Sound in the Binary Mixtures of Ethyl Chloroacetate + Cyclohexanone, + Chlorobenzene, + Bromobenzene, or + Benzyl Alcohol at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je0201828
Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K:	https://www.doi.org/10.1016/j.jct.2015.12.027
Thermodynamics of solvation in propylene glycol and methyl	https://www.doi.org/10.1016/j.jct.2014.06.006
Excess Volumes of Binary Solutions of Methyl Formate, Ethyl Formate, Propyl Formate, and Benzyl Acetate with Bromo-, Chloro-, and Nitrobenzenes at (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je700150e
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1683
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Measurement and correlation of the (p, ?, T) relation of liquid n-heptane, n-nonane, 2,4-dichlorotoluene, and bromobenzene in the temperature range from (283.15 to 473.15) K at pressures up to 30 MPa for use as density reference liquids:	https://www.doi.org/10.1016/j.jct.2008.02.020
Liquid-Liquid Equilibria in Binary Mixtures Containing Chlorobenzene, Bromobenzene, and Iodobenzene with ... methylimidazolim ... ylsulfonyl)imide:	https://www.doi.org/10.1021/je801005y
Activity coefficients and excess Gibbs energy of binary mixtures of N,N-dimethylformamide with selected compounds at 95.5 kPa:	https://www.doi.org/10.1016/j.fluid.2008.07.018
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1683
Thermophysical Properties For Diethylene Glycol + Nitrobenzene and Triethylene Glycol + (Chloro-, Bromo-, Nitro-) Benzene Systems at Different Temperatures:	https://www.doi.org/10.1007/s10765-008-0399-8
Thermophysical properties of the binary mixtures of 1,2-Dichloroethane with chlorobenzene and bromobenzene from 298.15 to 313.15 K:	https://www.doi.org/10.1021/je100552a
Studies on the importance of nature of substituent on the thermodynamic and transport properties of liquid mixtures at various temperatures:	https://www.doi.org/10.1016/j.jct.2016.05.015
Activity coefficients at infinite dilution of organic solutes in 1-hexyl-3-methylimidazolium trifluoroacetate and influence of interfacial adsorption using gas liquid chromatography:	https://www.doi.org/10.1016/j.jct.2013.10.038

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fpo:	Flash Point (Open Cup Method)

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter