Propane, 1,3-dibromo-

Other names:	1,3-Dibromopropane
	CH2BrCH2CH2Br
	Dibromo-1,3 propane
	TRIMETHYLENE DIBROMIDE
	Trimethylene bromide
	«alpha»,«gamma»-Dibromopropane
	«omega»,«omega»'-Dibromopropane
	Â«alphaÂ»,Â«gammaÂ»-Dibromopropane
	Â«omegaÂ»,Â«omegaÂ»'-Dibromopropane
Inchi:	InChI=1S/C3H6Br2/c4-2-1-3-5/h1-3H2
InchiKey:	VEFLKXRACNJHOV-UHFFFAOYSA-N
Formula:	C3H6Br2
SMILES:	BrCCCBr
Mol. weight [g/mol]:	201.89
CAS:	109-64-8

Physical Properties

Property code	Value	Unit	Source
gf	3.02	kJ/mol	Joback Method
hf	-52.59	kJ/mol	Joback Method
hfus	14.10	kJ/mol	Joback Method
hvap	47.60	kJ/mol	NIST Webbook
hvap	47.45 ± 0.10	kJ/mol	NIST Webbook
hvap	45.30	kJ/mol	NIST Webbook
hvap	47.46	kJ/mol	NIST Webbook
ie	10.26	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.07 ± 0.02	eV	NIST Webbook
log10ws	-2.08		Aqueous Solubility Prediction Method
logp	2.166		Crippen Method
mcvol	88.130	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
rinpol	963.70		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	936.00		NIST Webbook

rinpol	937.70		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	971.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1422.00		NIST Webbook
tb	440.05	K	KDB
tc	608.96	K	Joback Method
tf	238.65	K	KDB
tf	238.85 ± 0.50	K	NIST Webbook
tf	237.00 ± 0.40	K	NIST Webbook
tf	238.95 ± 0.60	K	NIST Webbook
tf	239.10	K	Aqueous Solubility Prediction Method
tt	238.60 ± 0.20	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.47	J/mol×K	400.36	Joback Method
cpg	155.22	J/mol×K	608.96	Joback Method
cpg	150.75	J/mol×K	574.20	Joback Method
cpg	145.98	J/mol×K	539.43	Joback Method
cpg	140.89	J/mol×K	504.66	Joback Method
cpg	135.46	J/mol×K	469.89	Joback Method
cpg	129.66	J/mol×K	435.13	Joback Method
cpl	167.44	J/mol×K	327.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	171.13	J/mol×K	352.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	171.36	J/mol×K	354.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	171.51	J/mol×K	355.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.70	J/mol×K	298.15	NIST Webbook
cpl	156.10	J/mol×K	245.70	NIST Webbook
cpl	159.00	J/mol×K	298.00	NIST Webbook
cpl	170.90	J/mol×K	351.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	170.68	J/mol×K	349.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	170.45	J/mol×K	348.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	170.23	J/mol×K	346.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	170.00	J/mol×K	345.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	169.78	J/mol×K	343.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	169.56	J/mol×K	342.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	169.35	J/mol×K	340.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	168.91	J/mol×K	337.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	168.70	J/mol×K	336.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	168.49	J/mol×K	334.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	168.27	J/mol×K	333.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	168.06	J/mol×K	331.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	167.86	J/mol×K	330.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	167.65	J/mol×K	328.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	162.24	J/mol×K	285.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	162.41	J/mol×K	286.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	162.57	J/mol×K	288.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	162.74	J/mol×K	289.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	162.92	J/mol×K	291.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.09	J/mol×K	292.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.26	J/mol×K	294.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	163.44	J/mol×K	295.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.62	J/mol×K	297.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.73	J/mol×K	298.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.79	J/mol×K	298.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	163.97	J/mol×K	300.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	164.15	J/mol×K	301.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	164.34	J/mol×K	303.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	164.52	J/mol×K	304.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	164.71	J/mol×K	306.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	164.89	J/mol×K	307.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	165.08	J/mol×K	309.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	165.27	J/mol×K	310.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	165.46	J/mol×K	312.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	165.65	J/mol×K	313.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	165.85	J/mol×K	315.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	166.04	J/mol×K	316.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	166.24	J/mol×K	318.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	166.43	J/mol×K	319.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	166.63	J/mol×K	321.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	166.83	J/mol×K	322.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	167.04	J/mol×K	324.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	167.24	J/mol×K	325.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	169.13	J/mol×K	339.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
dvisc	0.0004696	Pa×s	400.36	Joback Method
dvisc	0.0019272	Pa×s	269.37	Joback Method
dvisc	0.0013146	Pa×s	295.57	Joback Method
dvisc	0.0009544	Pa×s	321.76	Joback Method
dvisc	0.0007271	Pa×s	347.96	Joback Method
dvisc	0.0005754	Pa×s	374.16	Joback Method
dvisc	0.0030679	Pa×s	243.17	Joback Method
hfust	14.64	kJ/mol	238.60	NIST Webbook
hfust	14.64	kJ/mol	238.60	NIST Webbook
hfust	14.64	kJ/mol	238.60	NIST Webbook
hvapt	46.10 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	46.60	kJ/mol	372.00	NIST Webbook
hvapt	46.70 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	44.80 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	45.50 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	47.80	kJ/mol	419.00	NIST Webbook
hvapt	47.30 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	47.89	kJ/mol	439.40	NIST Webbook

rfi	1.52040		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II: HE m and V E m for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1 - x)a,x-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, a = 1 and v = x = 2 to 6
rhol	1980.22	kg/m3	292.55	Thermodynamic and Acoustic Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the Temperature Range From 293K to 313K at Pressures up to 100MPa
rhol	1970.22	kg/m3	297.98	Thermodynamic and Acoustic Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the Temperature Range From 293K to 313K at Pressures up to 100MPa
rhol	1961.58	kg/m3	303.07	Thermodynamic and Acoustic Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the Temperature Range From 293K to 313K at Pressures up to 100MPa
rhol	1952.84	kg/m3	308.02	Thermodynamic and Acoustic Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the Temperature Range From 293K to 313K at Pressures up to 100MPa

rhol	1941.18	kg/m3	314.58	Thermodynamic and Acoustic Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the Temperature Range From 293K to 313K at Pressures up to 100MPa
sfust	61.40	J/mol×K	238.60	NIST Webbook
srf	0.04	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	298.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	293.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61869e+01
Coeff. B	-4.23517e+03
Coeff. C	-6.39080e+01
Temperature range (K), min.	330.28
Temperature range (K), max.	467.14

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.97029e+01
Coeff. B	-6.17431e+03
Coeff. C	-3.53806e+00
Coeff. D	2.40591e-06
Temperature range (K), min.	283.15
Temperature range (K), max.	441.15

Sources

The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes: Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the temperature range from 293K to 313K at Pressures up to 100MPa.	https://www.doi.org/10.1016/j.jct.2018.12.042
Thermodynamic and Acoustic Properties of 1,3-Dibromopropane and 1,5-Dibromopentane within the Temperature Range From 293K to 313K and Pressures up to 100MPa.	https://www.doi.org/10.1007/s10765-009-0610-6
Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) VI: Hexyl {xC(u-1)H(2u-1)CO2CH3 + (1-x)alpha,omega-BrCH2(CH2)(v-2)CH2Br}, where u = 1 to 5, alpha = 1 and v = 2 to 20 binary mixtures	https://www.doi.org/10.1016/j.jct.2006.05.004
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109648&Units=SI
Gripper Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of (alkyl esters + alpha,beta-alkyl dihalides) VI.H and V for 20 binary mixtures	https://www.doi.org/10.1016/j.jct.2009.05.006
Thermodynamic study of (alkyl esters + a,w-alkyl dihalides) II. HE m and V E m for {xC(u-1)H2u-1CO2C2H5 + (1 x)alpha,omega-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1, and v = 2 to 6.	https://www.doi.org/10.1016/j.jct.2005.07.009
Vapor Pressure Data	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1586
Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 359.15) K:	https://www.doi.org/10.1021/je201002j
Joback Method	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1586.mol
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
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
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume