

# Propane, 1,3-dibromo-

<b>Other names:</b>	1,3-Dibromopropane CH <sub>2</sub> BrCH <sub>2</sub> CH <sub>2</sub> Br Dibromo-1,3 propane TRIMETHYLENE DIBROMIDE Trimethylene bromide «alpha», «gamma»-Dibromopropane «omega», «omega»'-Dibromopropane Δ«alphaΔ», Δ«gammaΔ»-Dibromopropane Δ«omegaΔ», Δ«omegaΔ»'-Dibromopropane
<b>Inchi:</b>	InChI=1S/C3H6Br <sub>2</sub> /c4-2-1-3-5/h1-3H2
<b>InchiKey:</b>	VEFLKXRACNJHOV-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>3</sub> H <sub>6</sub> Br <sub>2</sub>
<b>SMILES:</b>	BrCCCBr
<b>Mol. weight [g/mol]:</b>	201.89
<b>CAS:</b>	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	47.46	kJ/mol	NIST Webbook
hvap	47.60	kJ/mol	NIST Webbook
hvap	45.30	kJ/mol	NIST Webbook
hvap	47.45 ± 0.10	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	936.00		NIST Webbook
rinpol	937.70		NIST Webbook
rinpol	963.70		NIST Webbook
rinpol	955.00		NIST Webbook

rinpol	989.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	919.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1419.00		NIST Webbook
tb	440.05	K	KDB
tc	608.96	K	Joback Method
tf	238.85 ± 0.50	K	NIST Webbook
tf	238.65	K	KDB
tf	239.10	K	Aqueous Solubility Prediction Method
tf	238.95 ± 0.60	K	NIST Webbook
tf	237.00 ± 0.40	K	NIST Webbook
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	150.75	J/mol×K	574.20	Joback Method
cpg	155.22	J/mol×K	608.96	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
cpg	123.47	J/mol×K	400.36	Joback Method
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	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	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	159.00	J/mol×K	298.00	NIST Webbook

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	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
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	168.27	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	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	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	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	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	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
dvisc	0.0030679	Paxs	243.17	Joback Method
dvisc	0.0005754	Paxs	374.16	Joback Method
dvisc	0.0007271	Paxs	347.96	Joback Method
dvisc	0.0009544	Paxs	321.76	Joback Method
dvisc	0.0013146	Paxs	295.57	Joback Method
dvisc	0.0019272	Paxs	269.37	Joback Method
dvisc	0.0004696	Paxs	400.36	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	47.80	kJ/mol	419.00	NIST Webbook
hvapt	47.30 ± 0.10	kJ/mol	308.00	NIST Webbook
hvapt	46.70 ± 0.10	kJ/mol	315.00	NIST Webbook
hvapt	46.10 ± 0.10	kJ/mol	323.00	NIST Webbook
hvapt	45.50 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	44.80 ± 0.10	kJ/mol	338.00	NIST Webbook
hvapt	46.60	kJ/mol	372.00	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	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
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

rh0l	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
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	293.15	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	303.15	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

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vp}}) = A + B/(T + C)$
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
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Property code	pvap
Equation	$\ln(P_{\text{vap}}) = A + B/T + C*\ln(T) + D*T^2$
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

KDB:

<https://www.cheric.org/files/research/kdb/mol/mol1586.mol>

Thermodynamic study of (alkyl esters + alpha,beta-alkyl dihalides) VI: H and V

NIST Webbook

<https://www.doi.org/10.1016/j.jct.2009.05.006>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C109648&Units=SI>

(xCu-1H2u-1CO2(CH2)3CH3 + (1 - x)alpha,omega-BuCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1 and v = 0 to 6;

Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) II: HE m and V E m

Correlation Method

{xCu-1H2u-1CO2C2H5 + (1 - x)alpha,BuCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1 and v = 0 to 6;

alpha,omega-alkyl dihalogenoalkyl esters + alpha,omega-alkyl dihalides) IV: Hexane

and Hexadecane binary mixtures

Properties of 1,1-Dichloropropane and 1,1-Dibromoethane Handbook Yaws, Pressure Range From 293 K to 313 K

Temperature Range From 293 K to 313 K

alpha > 240 up to 100MPa:

Heat Capacity of

alpha,omega-Bromochloroalkanes and

Aqueous Solubility: Prigogine Method on the Hydrocarbon Chain Length and

McGowan Method: Temperature (283.15 to 355.15) K:

<https://www.doi.org/10.1016/j.jct.2005.07.009>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.doi.org/10.1016/j.jct.2018.12.042>

Properties of

alpha,omega-alkyl dihalides +

alpha,omega-alkyl dihalogenoalkyl esters +

alpha,omega-alkyl dihalides) IV: Hexane

and Hexadecane binary mixtures

Properties of 1,1-Dichloropropane and

1,1-Dibromoethane Handbook Yaws,

Pressure Range From 293 K to 313 K

Temperature Range From 293 K to 313 K

alpha > 240 up to 100MPa:

<https://www.doi.org/10.1007/s10765-009-0610-6>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<https://www.doi.org/10.1021/je201002j>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

<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

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rfi:</b>	Refractive Index
<b>rhol:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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