

# Propane, 1-bromo-3-chloro-

<b>Other names:</b>	1,3-Chbp 1-Bromo-3-chloropropane 1-Chloro-3-bromopropane 3-Bromo-1-chloropropane 3-Bromopropyl chloride 3-Chloro-1-bromopropane 3-Chloropropyl bromide NSC 9183 Trimethylene bromide chloride Trimethylene chlorobromide UN 2688 «omega»-Chlorobromopropane Â«omegaÂ»-Chlorobromopropane
<b>Inchi:</b>	InChI=1S/C3H6BrCl/c4-2-1-3-5/h1-3H2
<b>InchiKey:</b>	MFESCIUQSIBMSM-UHFFFAOYSA-N
<b>Formula:</b>	C3H6BrCl
<b>SMILES:</b>	C1CCCB1
<b>Mol. weight [g/mol]:</b>	157.44
<b>CAS:</b>	109-70-6

## Physical Properties

Property code	Value	Unit	Source
gf	-23.23	kJ/mol	Joback Method
hf	-94.66	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	44.06	kJ/mol	NIST Webbook
hvap	44.04 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.85		Aqueous Solubility Prediction Method
logp	2.010		Crippen Method
mcvol	82.870	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
rinpol	869.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	849.20		NIST Webbook
rinpol	869.50		NIST Webbook
rinpol	841.00		NIST Webbook

rinpol	830.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	416.00	K	NIST Webbook
tb	416.50	K	NIST Webbook
tb	415.50 ± 0.50	K	NIST Webbook
tb	416.50	K	NIST Webbook
tb	417.50 ± 0.50	K	NIST Webbook
tb	417.00 ± 4.00	K	NIST Webbook
tc	567.20	K	Joback Method
tf	214.30 ± 0.02	K	NIST Webbook
tf	214.20	K	Aqueous Solubility Prediction Method
vc	0.315	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.83	J/mol×K	371.63	Joback Method
cpg	148.53	J/mol×K	567.20	Joback Method
cpg	143.95	J/mol×K	534.60	Joback Method
cpg	139.10	J/mol×K	502.01	Joback Method
cpg	133.98	J/mol×K	469.41	Joback Method
cpg	128.57	J/mol×K	436.82	Joback Method
cpg	122.86	J/mol×K	404.22	Joback Method
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	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	170.00	J/molxK	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	170.23	J/molxK	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	170.45	J/molxK	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	170.68	J/molxK	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	170.90	J/molxK	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	171.13	J/molxK	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/molxK	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	169.78	J/molxK	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	162.41	J/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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	169.35	J/molxK	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	165.08	J/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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	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	167.65	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	167.86	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	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	168.27	J/molxK	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	168.49	J/molxK	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	168.70	J/molxK	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	168.91	J/molxK	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	169.13	J/molxK	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	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	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
dvisc	0.0012949	Paxs	266.07	Joback Method
dvisc	0.0019988	Paxs	239.68	Joback Method
dvisc	0.0004225	Paxs	371.63	Joback Method
dvisc	0.0005243	Paxs	345.24	Joback Method
dvisc	0.0006742	Paxs	318.85	Joback Method
dvisc	0.0009073	Paxs	292.46	Joback Method
dvisc	0.0034352	Paxs	213.29	Joback Method
hvapt	42.00	kJ/mol	407.00	NIST Webbook
hvapt	37.55	kJ/mol	416.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44017e+01
Coeff. B	-3.50342e+03
Coeff. C	-5.79010e+01
Temperature range (K), min.	306.12
Temperature range (K), max.	443.91

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Heat Capacity of alpha,omega-Bromochloroalkanes and alpha,bromochloroalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K.</b>	<a href="https://www.doi.org/10.1021/je201002j">https://www.doi.org/10.1021/je201002j</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C109706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109706&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvac:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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