

# Nonane, 1-bromo-

<b>Other names:</b>	1-Bromononane 1-NONYL BROMIDE 1-n-Nonyl bromide N-NONYL BROMIDE Nonyl bromide n-Nonyl-1-bromide
<b>Inchi:</b>	InChI=1S/C9H19Br/c1-2-3-4-5-6-7-8-9-10/h2-9H2,1H3
<b>InchiKey:</b>	AYMUQTNXKPEMLM-UHFFFAOYSA-N
<b>Formula:</b>	C9H19Br
<b>SMILES:</b>	CCCCCCCCCBr
<b>Mol. weight [g/mol]:</b>	207.15
<b>CAS:</b>	693-58-3

## Physical Properties

Property code	Value	Unit	Source
gf	39.22	kJ/mol	Joback Method
hf	-202.76	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.132		Crippen Method
mcvol	155.170	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1238.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1496.00		NIST Webbook
tb	474.20	K	NIST Webbook
tb	474.00	K	NIST Webbook
tc	650.81	K	Joback Method

tf	244.15	K	KDB
tf	244.20 ± 0.20	K	NIST Webbook
tf	242.40 ± 0.20	K	NIST Webbook
tf	244.09 ± 0.25	K	NIST Webbook
tf	242.44 ± 0.15	K	NIST Webbook
vc	0.602	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.03	J/mol×K	471.48	Joback Method
cpg	394.99	J/mol×K	650.81	Joback Method
cpg	383.88	J/mol×K	620.92	Joback Method
cpg	372.25	J/mol×K	591.03	Joback Method
cpg	360.07	J/mol×K	561.15	Joback Method
cpg	347.32	J/mol×K	531.26	Joback Method
cpg	333.98	J/mol×K	501.37	Joback Method
cpl	318.70	J/mol×K	321.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	325.00	J/mol×K	336.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	324.63	J/mol×K	334.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	310.56	J/mol×K	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	323.32	J/mol×K	331.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	326.99	J/mol×K	339.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	328.13	J/mol×K	341.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	329.39	J/mol×K	344.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	330.49	J/mol×K	346.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	331.79	J/mol×K	349.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	333.04	J/mol×K	351.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	333.74	J/mol×K	353.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	308.30	J/mol×K	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	322.16	J/mol×K	329.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	312.82	J/mol×K	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	315.10	J/mol×K	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	317.36	J/mol×K	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	319.61	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	321.87	J/mol×K	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	324.15	J/mol×K	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	326.41	J/mol×K	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	328.67	J/mol×K	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	330.92	J/mol×K	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	333.20	J/mol×K	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	335.46	J/mol×K	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	337.72	J/mol×K	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	339.98	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	342.26	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	344.51	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	346.77	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	349.03	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	351.31	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	353.57	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	320.96	J/mol×K	326.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	358.08	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	360.36	J/mol×K	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	362.62	J/mol×K	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	364.88	J/mol×K	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	302.55	J/mol×K	284.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	303.54	J/mol×K	286.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	304.62	J/mol×K	289.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis



cpl	305.57	J/mol×K	291.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	306.69	J/mol×K	294.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	307.68	J/mol×K	296.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	308.80	J/mol×K	299.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	309.82	J/mol×K	301.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	310.95	J/mol×K	304.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	311.91	J/mol×K	306.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	313.01	J/mol×K	309.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	314.10	J/mol×K	311.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	315.18	J/mol×K	314.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	316.32	J/mol×K	316.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	317.44	J/mol×K	319.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	355.82	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	319.80	J/molxK	324.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
dvisc	0.0002865	Paxs	471.48	Joback Method
dvisc	0.0003711	Paxs	434.73	Joback Method
dvisc	0.0005042	Paxs	397.98	Joback Method
dvisc	0.0007290	Paxs	361.24	Joback Method
dvisc	0.0011459	Paxs	324.49	Joback Method
dvisc	0.0020219	Paxs	287.74	Joback Method
dvisc	0.0042127	Paxs	250.99	Joback Method
hfust	30.12	kJ/mol	243.20	NIST Webbook
hfust	30.12	kJ/mol	243.20	NIST Webbook
hvapt	53.10	kJ/mol	450.50	NIST Webbook
hvapt	52.20	kJ/mol	470.00	NIST Webbook
speedsl	1329.91	m/s	253.46	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1262.72	m/s	273.29	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1101.12	m/s	323.14	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	1009.85	m/s	353.10	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	921.46	m/s	383.05	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	808.79	m/s	422.72	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	864.42	m/s	402.98	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1165.07	m/s	303.15	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.76688e+01
Coeff. B	-5.16229e+03
Coeff. C	-7.86350e+01
Temperature range (K), min.	375.64

Temperature range (K), max.	496.39
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Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.69072e+01
Coeff. B	-1.03437e+04
Coeff. C	-1.17047e+01
Coeff. D	5.06259e-06
Temperature range (K), min.	391.15
Temperature range (K), max.	549.15

## Sources

- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K:** <https://www.doi.org/10.1021/je900227j>
- KDB Vapor Pressure Data:** <https://www.thermo.com/files/research/kdb/mol/mol1649.mol>
- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>
- Joback Method:** [https://en.wikipedia.org/wiki/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>
- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C693583&Units=SI>
- Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)
- KDB Vapor Pressure Data:** <https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1649>
- Isobaric heat capacity, isothermal compressibility and fluctuational heat capacities of 1-bromoalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis:** <https://www.doi.org/10.1007/s10765-016-2064-y>
- <https://www.doi.org/10.1021/je049652j>

## 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

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>speedsl:</b>	Speed of sound in fluid
<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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