

Nonane, 1-bromo-

Other names:	1-Bromononane 1-NONYL BROMIDE 1-n-Nonyl bromide N-NONYL BROMIDE Nonyl bromide n-Nonyl-1-bromide
Inchi:	InChI=1S/C9H19Br/c1-2-3-4-5-6-7-8-9-10/h2-9H2,1H3
InchiKey:	AYMUQTNXKPEMLM-UHFFFAOYSA-N
Formula:	C9H19Br
SMILES:	CCCCCCCCCBr
Mol. weight [g/mol]:	207.15
CAS:	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	1231.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1476.00		NIST Webbook
tb	474.00	K	NIST Webbook
tb	474.20	K	NIST Webbook
tc	650.81	K	Joback Method

tf	244.20 ± 0.20	K	NIST Webbook
tf	242.44 ± 0.15	K	NIST Webbook
tf	244.09 ± 0.25	K	NIST Webbook
tf	242.40 ± 0.20	K	NIST Webbook
tf	244.15	K	KDB
vc	0.602	m3/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	319.61	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
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/molxK	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/molxK	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/molxK	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/molxK	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	323.32	J/molxK	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	308.30	J/molxK	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	310.56	J/molxK	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	312.82	J/molxK	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	315.10	J/molxK	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	317.36	J/molxK	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	326.99	J/molxK	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	321.87	J/molxK	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	324.15	J/molxK	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	326.41	J/molxK	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	328.67	J/molxK	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	330.92	J/molxK	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	333.20	J/molxK	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	335.46	J/molxK	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	337.72	J/molxK	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	339.98	J/molxK	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	355.82	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	358.08	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	360.36	J/molxK	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	362.62	J/molxK	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	325.00	J/molxK	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	302.55	J/molxK	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/molxK	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/molxK	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
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cpl	305.57	J/molxK	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
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cpl	306.69	J/molxK	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
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cpl	307.68	J/molxK	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
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cpl	308.80	J/molxK	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
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cpl	309.82	J/molxK	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
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cpl	310.95	J/molxK	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
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cpl	311.91	J/molxK	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
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cpl	313.01	J/molxK	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
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cpl	314.10	J/molxK	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
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cpl	315.18	J/molxK	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
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cpl	316.32	J/molxK	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
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cpl	317.44	J/molxK	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
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cpl	318.70	J/molxK	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
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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
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cpl	320.96	J/molxK	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
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cpl	322.16	J/molxK	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	364.88	J/molxK	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	324.63	J/molxK	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
dvisc	0.0020219	Paxs	287.74	Joback Method
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	0.0042127	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	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

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	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	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	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	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

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

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1649.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693583&Units=SI
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
Speed of Sound, Densities, and Isentropic Compressibilities of Liquid Carbon Dioxide at Temperatures from (243.15 to 423.15) K:	https://www.doi.org/10.1021/je900227j
Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Pressure of 1-bromoalkanes:	https://www.doi.org/10.1007/s10765-016-2064-y
KDB Vapor Pressure Data:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1649
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:	https://en.wikipedia.org/wiki/Joback_method
	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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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