

Decane, 1-bromo-

Other names:	1-Bromodecane 1-Decyl bromide Decyl bromide N-DECYL BROMIDE
Inchi:	InChI=1S/C10H21Br/c1-2-3-4-5-6-7-8-9-10-11/h2-10H2,1H3
InchiKey:	MYMSJFSSOOQERIO-UHFFFAOYSA-N
Formula:	C10H21Br
SMILES:	CCCCCCCCCBr
Mol. weight [g/mol]:	221.18
CAS:	112-29-8

Physical Properties

Property code	Value	Unit	Source
gf	47.64	kJ/mol	Joback Method
hf	-223.40	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	74.77 ± 0.38	kJ/mol	NIST Webbook
log10ws	-4.44		Crippen Method
logp	4.522		Crippen Method
mcvol	169.260	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1344.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1578.00		NIST Webbook
tb	513.80	K	NIST Webbook
tb	511.00	K	NIST Webbook
tb	511.20	K	NIST Webbook

tc	672.07	K	Joback Method
tf	244.00 ± 0.30	K	NIST Webbook
tf	243.95	K	KDB
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.97	J/molxK	494.36	Joback Method
cpg	379.77	J/molxK	523.98	Joback Method
cpg	393.94	J/molxK	553.60	Joback Method
cpg	407.47	J/molxK	583.21	Joback Method
cpg	420.41	J/molxK	612.83	Joback Method
cpg	432.76	J/molxK	642.45	Joback Method
cpg	444.56	J/molxK	672.07	Joback Method
cpl	339.35	J/molxK	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	336.85	J/molxK	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	334.38	J/molxK	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	341.85	J/molxK	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	344.35	J/molxK	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	346.85	J/molxK	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	349.35	J/molxK	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	351.85	J/molxK	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	354.33	J/molxK	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	356.83	J/molxK	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	359.33	J/molxK	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	361.82	J/molxK	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	364.32	J/molxK	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	366.82	J/molxK	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	369.32	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	371.80	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	374.30	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	376.80	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	379.30	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	381.80	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	384.30	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	386.80	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	389.27	J/molxK	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	391.77	J/molxK	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	394.27	J/molxK	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	396.77	J/molxK	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	332.60	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	333.65	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	335.00	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	336.08	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	336.90	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	366.38	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
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cpl	339.29	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	340.37	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	341.48	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	342.74	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	343.89	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	345.13	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	346.34	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	347.51	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	348.84	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	350.10	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	351.41	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	352.71	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	354.02	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
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cpl	355.32	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
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cpl	356.14	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
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cpl	357.34	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
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cpl	359.30	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
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cpl	360.70	J/molxK	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
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cpl	362.13	J/molxK	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
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cpl	363.37	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
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cpl	364.86	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	338.20	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
cpl	367.07	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
dvisc	0.0002633	Paxs	494.36	Joback Method
dvisc	0.0019414	Paxs	300.94	Joback Method
dvisc	0.0010852	Paxs	339.63	Joback Method
dvisc	0.0006832	Paxs	378.31	Joback Method
dvisc	0.0041233	Paxs	262.26	Joback Method
dvisc	0.0003428	Paxs	455.68	Joback Method
dvisc	0.0004687	Paxs	416.99	Joback Method
hvapt	56.10	kJ/mol	468.00	NIST Webbook
hvapt	56.60	kJ/mol	476.50	NIST Webbook
speedsl	1123.81	m/s	323.20	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	1032.24	m/s	353.19	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	944.49	m/s	383.22	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	888.22	m/s	403.23	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	833.21	m/s	423.27	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.25 ± 0.25	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56804e+01
Coeff. B	-4.72600e+03

Coeff. C	-8.39720e+01
Temperature range (K), min.	391.00
Temperature range (K), max.	539.76

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.06974e+02
Coeff. B	-1.13131e+04
Coeff. C	-1.31064e+01
Coeff. D	5.57428e-06
Temperature range (K), min.	383.15
Temperature range (K), max.	570.15

Sources

Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-haloalkanes:

<https://www.doi.org/10.1007/s10765-016-2064-y>

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Joback Method:

https://www.chemeo.com/doc/models/crippen_log10ws

KDB:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<https://www.thermo.com/files/research/kdb/mol/mol1652.mol>

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C112298&Units=SI>

Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-haloalkanes at Temperatures and Pressures within the temperature range from 284.15 K to 393.15 K. A group additivity and molecular connectivity analysis:

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

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.doi.org/10.1021/je900227j>

<https://www.doi.org/10.1021/je049652j>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1652>

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
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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