

Dodecane, 1-bromo-

Other names:	1-Bromododecane Dodecyl bromide LAURYL BROMIDE N-DODECYL BROMIDE
Inchi:	InChI=1S/C12H25Br/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-12H2,1H3
InchiKey:	PBLNBZIONSLZBU-UHFFFAOYSA-N
Formula:	C12H25Br
SMILES:	CCCCCCCCCCBr
Mol. weight [g/mol]:	249.23
CAS:	143-15-7

Physical Properties

Property code	Value	Unit	Source
chl	-7950.30 ± 2.00	kJ/mol	NIST Webbook
gf	64.48	kJ/mol	Joback Method
hf	-269.90 ± 2.60	kJ/mol	NIST Webbook
hfl	-344.70 ± 2.60	kJ/mol	NIST Webbook
hfus	32.12	kJ/mol	Joback Method
hvap	74.77 ± 0.38	kJ/mol	NIST Webbook
hvap	74.80 ± 0.40	kJ/mol	NIST Webbook
hvap	74.77 ± 0.38	kJ/mol	NIST Webbook
hvap	74.77	kJ/mol	NIST Webbook
log10ws	-5.28		Crippen Method
logp	5.302		Crippen Method
mcvol	197.440	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1552.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	549.20	K	NIST Webbook
tc	714.73	K	Joback Method
tf	284.80	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.39	J/mol×K	540.12	Joback Method
cpg	547.70	J/mol×K	714.73	Joback Method
cpg	534.75	J/mol×K	685.63	Joback Method
cpg	521.20	J/mol×K	656.53	Joback Method
cpg	507.01	J/mol×K	627.42	Joback Method
cpg	492.16	J/mol×K	598.32	Joback Method
cpg	476.62	J/mol×K	569.22	Joback Method
cpl	448.72	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	476.50	J/mol×K	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	473.41	J/mol×K	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	470.32	J/mol×K	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	467.23	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	464.14	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	461.08	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	454.90	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	451.81	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	457.99	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	427.11	J/mol×K	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	430.20	J/mol×K	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	433.26	J/mol×K	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	436.35	J/mol×K	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	439.44	J/mol×K	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	442.53	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	399.29	J/mol×K	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	402.38	J/mol×K	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	405.47	J/mol×K	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	408.56	J/mol×K	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	411.65	J/mol×K	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	414.75	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	417.84	J/mol×K	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	420.93	J/mol×K	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	424.02	J/mol×K	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	445.62	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
dvisc	0.0009435	Paxs	369.91	Joback Method
dvisc	0.0005832	Paxs	412.46	Joback Method
dvisc	0.0003944	Paxs	455.01	Joback Method
dvisc	0.0002852	Paxs	497.57	Joback Method
dvisc	0.0002170	Paxs	540.12	Joback Method
dvisc	0.0017300	Paxs	327.35	Joback Method
dvisc	0.0038020	Paxs	284.80	Joback Method
hvapt	62.20	kJ/mol	510.50	NIST Webbook
rhol	952.40	kg/m3	393.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1048.50	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1039.80	kg/m3	293.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1035.60	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rhol	1014.00	kg/m3	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	996.20	kg/m3	343.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	979.00	kg/m3	363.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	923.70	kg/m3	423.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1056.50	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
speedsl	1323.54	m/s	273.32	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1224.75	m/s	303.21	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1161.16	m/s	323.18	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	1069.74	m/s	353.15	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	982.95	m/s	383.17	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	926.37	m/s	403.19	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	871.74	m/s	423.14	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	407.70	K	0.80	NIST Webbook
tbrp	473.30 ± 0.70	K	13.30	NIST Webbook
tbrp	365.50 ± 0.50	K	0.03	NIST Webbook

Correlations

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

Coeff. A	1.54636e+01
Coeff. B	-4.93910e+03
Coeff. C	-9.37860e+01
Temperature range (K), min.	419.24
Temperature range (K), max.	580.29

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vp}}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.11805e+02
Coeff. B	-1.24932e+04
Coeff. C	-1.36262e+01
Coeff. D	5.05498e-06
Temperature range (K), min.	411.15
Temperature range (K), max.	610.15

Sources

Speed of Sound, Densities, and Isentropic Compressibilities of Liquid KDB Vapor Pressure Data: Isobaric Pressures and Temperatures from (243.15 to 423.15) K: Crippen Method:

KDB:

NIST Webbook:

The Yaws Handbook of Vapor Pressure:

Isobaric heat capacity, isothermal compressibility and fluctuational densities of some fluorocarbenes within the Temperature Range from (243.15 to 423.15) K:

McGowan Method:

Joback Method:

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

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1654>

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

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<http://webbook.nist.gov/cgi/cbook.cgi?ID=C143157&Units=SI>

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

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

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

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

Legend

chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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
rhol:	Liquid Density
rinpol:	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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