

Undecane, 1-bromo-

Other names:	1-Bromoundecane N-UNDECYL BROMIDE Undecyl bromide n-Undecyl-1-bromide
Inchi:	InChI=1S/C11H23Br/c1-2-3-4-5-6-7-8-9-10-11-12/h2-11H2,1H3
InchiKey:	IKPSIIXIDAQLG-UHFFFAOYSA-N
Formula:	C11H23Br
SMILES:	CCCCCCCCCCCCBr
Mol. weight [g/mol]:	235.20
CAS:	693-67-4

Physical Properties

Property code	Value	Unit	Source
gf	56.06	kJ/mol	Joback Method
hf	-244.04	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	46.52	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.912		Crippen Method
mcvol	183.350	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1449.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1687.00		NIST Webbook
tb	517.24	K	Joback Method
tc	693.35	K	Joback Method
tf	263.25	K	KDB
tf	263.30 ± 0.30	K	NIST Webbook
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.78	J/mol×K	517.24	Joback Method
cpg	495.48	J/mol×K	693.35	Joback Method
cpg	470.08	J/mol×K	634.65	Joback Method
cpg	456.47	J/mol×K	605.30	Joback Method
cpg	442.24	J/mol×K	575.94	Joback Method
cpg	427.35	J/mol×K	546.59	Joback Method
cpg	483.07	J/mol×K	664.00	Joback Method
cpl	435.50	J/mol×K	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	423.06	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	425.56	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	433.01	J/mol×K	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	428.02	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	420.57	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	430.52	J/mol×K	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	373.22	J/mol×K	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	375.72	J/mol×K	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	378.21	J/mol×K	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	380.70	J/mol×K	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	383.19	J/mol×K	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	415.58	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	388.18	J/mol×K	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	390.67	J/mol×K	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	

cpl	393.17	J/mol×K	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	395.66	J/mol×K	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	398.15	J/mol×K	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	400.62	J/mol×K	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	403.12	J/mol×K	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	405.61	J/mol×K	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	408.10	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	410.60	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	413.09	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	385.69	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	418.08	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
dvisc	0.0018422	Pa×s	314.15	Joback Method
dvisc	0.0010167	Pa×s	354.77	Joback Method
dvisc	0.0006340	Pa×s	395.38	Joback Method
dvisc	0.0003139	Pa×s	476.62	Joback Method
dvisc	0.0002399	Pa×s	517.24	Joback Method
dvisc	0.0039826	Pa×s	273.53	Joback Method
dvisc	0.0004317	Pa×s	436.00	Joback Method
hfust	33.47	kJ/mol	263.30	NIST Webbook
hfust	33.47	kJ/mol	263.30	NIST Webbook
hvapt	59.50	kJ/mol	494.50	NIST Webbook
hvapt	58.80	kJ/mol	485.50	NIST Webbook
speedsl	1054.42	m/s	353.14	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1145.61	m/s	323.19	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1208.99	m/s	303.22	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	1307.02	m/s	273.42	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	909.71	m/s	403.13	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	966.59	m/s	383.14	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	854.45	m/s	423.13	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	410.70	K	2.40	NIST Webbook
tbrp	415.00	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61805e+01

Coeff. B	-5.03056e+03
Coeff. C	-8.90320e+01
Temperature range (K), min.	405.56
Temperature range (K), max.	551.87

Sources

Isobaric heat capacity, isothermal compressibility and fluctuational properties of Solid Densities and Isentropic Compressibilities of Liquid Carbon Monoxide at Temperatures from (243.15 to 423.15) K: NIST Webbook:

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

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C693674&Units=SI>

The Yaws Handbook of Vapor Pressure:
Crippen Method:

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

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

Joback Method:

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

KDB:

<https://www.cheric.org/files/research/kdb/mol/mol1653.mol>

McGowan Method:

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

Legend

cp_g:	Ideal gas heat capacity
cp_l:	Liquid phase heat capacity
dv_{isc}:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hf_{us}:	Enthalpy of fusion at standard conditions
hf_{ust}:	Enthalpy of fusion at a given temperature
h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
p_{vap}:	Vapor pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
speed_{sl}:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tb_{rp}:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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