

Pentane, 1-bromo-

Other names:	1-BROMOPENTANE 1-Pentyl bromide Amyl bromide N-AMYL BROMIDE PENTYLBROMIDE Pentyl bromide n-C ₅ H ₁₁ Br n-Pentyl bromide
Inchi:	InChI=1S/C ₅ H ₁₁ Br/c1-2-3-4-5-6/h2-5H ₂ ,1H ₃
InchiKey:	YZWKKMVJZFACSU-UHFFFAOYSA-N
Formula:	C ₅ H ₁₁ Br
SMILES:	CCCCCBr
Mol. weight [g/mol]:	151.04
CAS:	110-53-2

Physical Properties

Property code	Value	Unit	Source
af	0.3840		KDB
chl	-3369.40 ± 1.40	kJ/mol	NIST Webbook
gf	5.54	kJ/mol	Joback Method
hf	-129.80 ± 1.90	kJ/mol	NIST Webbook
hfl	-170.40 ± 1.50	kJ/mol	NIST Webbook
hfus	13.99	kJ/mol	Joback Method
hvap	33.16	kJ/mol	Joback Method
ie	10.10 ± 0.02	eV	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
ie	10.01	eV	NIST Webbook
log10ws	-3.07		Aqueous Solubility Prediction Method
log10ws	-3.08		Estimated Solubility Method
logp	2.571		Crippen Method
mvol	98.810	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3770.00	kPa	KDB

rinpol	810.20		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	807.70		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	809.70		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	810.90		NIST Webbook
rinpol	808.50		NIST Webbook
rinpol	807.70		NIST Webbook
rinpol	806.50		NIST Webbook
rinpol	833.80		NIST Webbook
rinpol	832.70		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	817.70		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	809.70		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	843.60		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	830.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1052.00		NIST Webbook
ripol	1055.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1068.00		NIST Webbook
sl	406.77	J/molxK	NIST Webbook
tb	402.70	K	KDB
tb	391.80 ± 1.50	K	NIST Webbook
tb	391.10 ± 0.60	K	NIST Webbook
tb	402.73 ± 0.15	K	NIST Webbook
tb	402.70 ± 0.40	K	NIST Webbook

tb	402.00 ± 0.40	K	NIST Webbook
tb	402.90	K	NIST Webbook
tb	402.80	K	NIST Webbook
tb	403.00	K	NIST Webbook
tb	391.40 ± 0.50	K	NIST Webbook
tc	564.80	K	KDB
tf	185.00	K	KDB
tf	180.48	K	Aqueous Solubility Prediction Method
tf	185.20 ± 0.20	K	NIST Webbook
tf	184.80 ± 5.00	K	NIST Webbook
tf	178.48 ± 0.20	K	NIST Webbook
tf	185.10 ± 0.20	K	NIST Webbook
vc	0.378	m ³ /kmol	KDB
zc	0.3030590		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.36	J/mol×K	379.96	Joback Method
cpg	211.43	J/mol×K	564.76	Joback Method
cpg	204.02	J/mol×K	533.96	Joback Method
cpg	196.26	J/mol×K	503.16	Joback Method
cpg	188.13	J/mol×K	472.36	Joback Method
cpg	179.61	J/mol×K	441.56	Joback Method
cpg	170.69	J/mol×K	410.76	Joback Method
cpl	194.86	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	207.05	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	199.09	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	198.35	J/mol×K	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
cpl	197.61	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	196.98	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	196.21	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	195.60	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	171.59	J/mol×K	290.70	NIST Webbook
cpl	174.90	J/mol×K	206.60	NIST Webbook
cpl	219.70	J/mol×K	298.15	NIST Webbook
cpl	206.69	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	205.89	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	199.80	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	205.07	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	200.47	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	201.48	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	201.57	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	202.76	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	203.58	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	187.88	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	188.46	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	189.17	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	189.85	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	190.33	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	190.94	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	191.57	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	192.17	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	193.01	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
cpl	193.53	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
cpl	194.17	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
cpl	204.33	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
dvisc	0.0004529	Paxs	350.95	Joback Method
dvisc	0.0012330	Paxs	263.93	Joback Method
dvisc	0.0008265	Paxs	292.94	Joback Method
dvisc	0.0005954	Paxs	321.94	Joback Method
dvisc	0.0020303	Paxs	234.92	Joback Method
dvisc	0.0038476	Paxs	205.91	Joback Method

dvisc	0.0003591	Paxs	379.96	Joback Method
hfust	11.46	kJ/mol	185.10	NIST Webbook
hfust	14.36	kJ/mol	185.10	NIST Webbook
hfust	14.37	kJ/mol	185.10	NIST Webbook
hfust	14.37	kJ/mol	185.10	NIST Webbook
hvapt	34.48	kJ/mol	402.70	KDB
hvapt	41.00	kJ/mol	368.00	NIST Webbook
hvapt	35.01	kJ/mol	402.90	NIST Webbook
rho1	1208.50	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1260.30	kg/m3	253.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1249.90	kg/m3	263.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1214.90	kg/m3	293.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1083.40	kg/m3	393.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1097.40	kg/m3	383.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1124.70	kg/m3	363.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rho1	1151.00	kg/m ³	343.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1177.10	kg/m ³	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1239.60	kg/m ³	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
sfust	62.00	J/mol×K	185.10	NIST Webbook
sfust	77.61	J/mol×K	185.10	NIST Webbook
sfust	77.60	J/mol×K	185.10	NIST Webbook
speedsl	666.58	m/s	423.48	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1240.04	m/s	243.73	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1037.13	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	972.37	m/s	323.17	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	877.57	m/s	353.18	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	785.49	m/s	383.23	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	725.54	m/s	403.28	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1137.50	m/s	273.32	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	294.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.74893e+01
Coeff. B	-5.01695e+03

Coeff. C	-9.21200e+00
Temperature range (K), min.	300.87
Temperature range (K), max.	421.19

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.04728e+02
Coeff. B	-1.21476e+04
Coeff. C	-2.91790e+01
Coeff. D	3.11793e-05
Temperature range (K), min.	294.15
Temperature range (K), max.	564.76

Sources

Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 298.15 to 423.15 K. Acentric Compressibilities of Liquid 1-chloroalkanes at Temperatures from (243.15 to 423.15) K: Joback Method:	https://www.doi.org/10.1021/je049652j
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 298.15 to 423.15 K. Acentric Compressibilities of Liquid 1-chloroalkanes at Temperatures from (243.15 to 423.15) K: Joback Method:	https://www.doi.org/10.1021/je900227j
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 298.15 to 423.15 K. Acentric Compressibilities of Liquid 1-chloroalkanes at Temperatures from (243.15 to 423.15) K: Joback Method:	https://www.thermo.com/files/research/kdb/mol/mol1620.mol
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 298.15 to 423.15 K. Acentric Compressibilities of Liquid 1-chloroalkanes at Temperatures from (243.15 to 423.15) K: Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1620
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110532&Units=SI
The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K: Prediction Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K: Prediction Method:	https://www.doi.org/10.1021/je700015t
Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K: Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpa:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
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
zc:	Critical Compressibility

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