Butane, 1,4-dibromo-

Other names:	1,4-Butylene bromide
	1,4-Dibrombutan
	1,4-Dibromobutane
	BrCH2CH2CH2CH2Br
	DBB
	Dibromo-1,4 butane
	TETRAMETHYLENE DIBROMIDE
Inchi:	InChI=1S/C4H8Br2/c5-3-1-2-4-6/h1-4H2
InchiKey:	ULTHEAFYOOPTTB-UHFFFAOYSA-N
Formula:	C4H8Br2
SMILES:	BrCCCCBr
Mol. weight [g/mol]:	215.91
CAS:	110-52-1

Physical Properties

Property code	Value	Unit	Source
gf	11.44	kJ/mol	Joback Method
hf	-85.98	kJ/mol	NIST Webbook
hfl	-140.10 ± 5.10	kJ/mol	NIST Webbook
hfus	16.69	kJ/mol	Joback Method
hvap	53.09	kJ/mol	NIST Webbook
hvap	52.60	kJ/mol	NIST Webbook
hvap	53.09 ± 0.12	kJ/mol	NIST Webbook
hvap	53.05	kJ/mol	NIST Webbook
ie	10.27	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.556		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1084.60		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1057.70		NIST Webbook

ripol	1559.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	470.20	K	NIST Webbook
tb	466.00 ± 3.00	K	NIST Webbook
tb	471.00 ± 3.00	K	NIST Webbook
tc	629.65	K	Joback Method
tf	252.10 ± 0.50	K	NIST Webbook
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.04	J/mol×K	423.24	Joback Method
cpg	198.06	J/mol×K	629.65	Joback Method
cpg	192.36	J/mol×K	595.25	Joback Method
cpg	186.31	J/mol×K	560.85	Joback Method
cpg	179.88	J/mol×K	526.45	Joback Method
cpg	173.04	J/mol×K	492.04	Joback Method
cpg	165.77	J/mol×K	457.64	Joback Method
cpl	190.32	J/mol×K	289.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	200.73	J/mol×K	348.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	201.03	J/mol×K	349.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	201.33	J/mol×K	351.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	201.63	J/mol×K	352.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	201.93	J/mol×K	354.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	202.14	J/mol×K	355.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	191.20	J/mol×K	298.15	NIST Webbook

cpl	189.62	J/mol×K	285.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	189.85	J/mol×K	286.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	190.08	J/mol×K	288.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	200.43	J/mol×K	346.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	190.55	J/mol×K	291.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	190.79	J/mol×K	292.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	191.03	J/mol×K	294.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	191.27	J/mol×K	295.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	191.52	J/mol×K	297.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	191.68	J/mol×K	298.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	191.76	J/mol×K	298.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	192.01	J/mol×K	300.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	192.26	J/mol×K	301.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	192.51	J/mol×K	303.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	192.76	J/mol×K	304.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	193.01	J/mol×K	306.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	193.26	J/mol×K	307.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	193.52	J/mol×K	309.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	193.78	J/mol×K	310.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	194.04	J/mol×K	312.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	194.30	J/mol×K	313.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	199.55	J/mol×K	342.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	194.82	J/mol×K	316.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	195.09	J/mol×K	318.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	195.35	J/mol×K	319.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	195.62	J/mol×K	321.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	195.89	J/mol×K	322.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	196.16	J/mol×K	324.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	196.44	J/mol×K	325.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	196.71	J/mol×K	327.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	196.99	J/mol×K	328.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	197.27	J/mol×K	330.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	197.55	J/mol×K	331.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	197.83	J/mol×K	333.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	198.11	J/mol×K	334.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	198.40	J/mol×K	336.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	198.68	J/mol×K	337.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	198.97	J/mol×K	339.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	200.14	J/mol×K	345.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	194.56	J/mol×K	315.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	199.84	J/mol×K	343.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	199.26	J/mol×K	340.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
dvisc	0.0004394	Pa×s	423.24	Joback Method
dvisc	0.0005429	Pa×s	395.11	Joback Method
dvisc	0.0006928	Pa×s	366.97	Joback Method
dvisc	0.0009206	Pa×s	338.84	Joback Method
dvisc	0.0012880	Pa×s	310.71	Joback Method
dvisc	0.0019266	Pa×s	282.57	Joback Method
dvisc	0.0031503	Pa×s	254.44	Joback Method
hvapt	49.40	kJ/mol	387.50	NIST Webbook
hvapt	51.40	kJ/mol	447.50	NIST Webbook
rfi	1.51630		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II: HE m and V E m for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1 - x)a,x-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, a = 1 and v = x = 2 to 6
srf	0.04	N/m	293.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	298.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

srf	0.04	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.20	K	0.80	NIST Webbook
tbrp	338.00	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51599e+01
Coeff. B	-4.23974e+03
Coeff. C	-6.80070e+01
Temperature range (K), min.	353.08
Temperature range (K), max.	498.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.74283e+01
Coeff. B	-1.01050e+04
Coeff. C	-1.17919e+01
Coeff. D	5.60527e-06
Temperature range (K), min.	375.15
Temperature range (K), max.	520.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K:	https://www.doi.org/10.1021/je201002j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1602
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110521&Units=SI
Thermodynamic study of (alkyl esters + alpha,beta-alkyl dihalides) VI.H and V for 20 binary mixtures {xCu-1H2u-1CO2(CH2)3CH3 + (1 - x)alpha,omega-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1, and v = omega = 2 to 6:	https://www.doi.org/10.1016/j.jct.2009.05.006
Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV. Hex and Vex for 25 binary mixtures {xC(u-1)H(2u-1)CO2CH3 + (1 - x)alpha,omega-BrCH2(CH2)(v-2)CH2Br}, where u = 1 to 5, alpha = 1 and v = omega = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.05.004
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1602.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes:	https://www.doi.org/10.1016/j.jct.2018.12.042
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II: HE m and V E m for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1 - x)a,x-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, a = 1 and v = x = 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.07.009

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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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