Butane, 1-bromo-

Other names: 1-BROMOBUTANE

BUTYL BROMIDE

UN 1126

n-Butyl bromide

n-C4H9Br

Inchi:InChI=1S/C4H9Br/c1-2-3-4-5/h2-4H2,1H3InchiKey:MPPPKRYCTPRNTB-UHFFFAOYSA-N

Formula: C4H9Br SMILES: CCCCBr Mol. weight [g/mol]: 137.02 CAS: 109-65-9

Physical Properties

Property code	Value	Unit	Source
af	0.3390		KDB
chl	-2716.50 ± 1.30	kJ/mol	NIST Webbook
gf	-2.88	kJ/mol	Joback Method
hf	-107.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-143.80 ± 1.30	kJ/mol	NIST Webbook
hfl	-148.00	kJ/mol	NIST Webbook
hfus	9.12	kJ/mol	Thermodynamics of Ionic Liquid Precursors. 1-Bromobutane and Its Isomers
hvap	36.70 ± 0.10	kJ/mol	NIST Webbook
hvap	36.40	kJ/mol	NIST Webbook
hvap	36.60 ± 0.10	kJ/mol	NIST Webbook
hvap	36.70 ± 0.10	kJ/mol	NIST Webbook
hvap	36.60 ± 0.10	kJ/mol	NIST Webbook
hvap	36.40	kJ/mol	NIST Webbook
hvap	36.71	kJ/mol	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
ie	10.13 ± 0.01	eV	NIST Webbook
ie	10.12	eV	NIST Webbook
ie	10.13 ± 0.01	eV	NIST Webbook
ie	10.13 ± 0.02	eV	NIST Webbook

log10ws	-2.37		Aqueous Solubility Prediction Method
log10ws	-2.37		Estimated Solubility Method
logp	2.181		Crippen Method
mcvol	84.720	ml/mol	McGowan Method
рс	4260.00	kPa	KDB
rinpol	732.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	740.50		NIST Webbook
rinpol	727.50		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	716.80		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	730.40		NIST Webbook
rinpol	731.40		NIST Webbook
rinpol	703.50		NIST Webbook
rinpol	705.40		NIST Webbook
rinpol	706.90		NIST Webbook
rinpol	712.20		NIST Webbook
rinpol	703.60		NIST Webbook
rinpol	701.90		NIST Webbook
rinpol	710.00		NIST Webbook
ripol	975.00		NIST Webbook
ripol	948.00		NIST Webbook
ripol	955.00		NIST Webbook
ripol	944.00		NIST Webbook

ZC	0.2892410		KDB
VC	0.322	m3/kmol	KDB
tf	160.40 ± 0.20	K	NIST Webbook
tf	160.80 ± 0.40	K	NIST Webbook
tf	160.70 ± 1.50	K	NIST Webbook
tf	385.40	K	NIST Webbook
tf	161.02	K	Aqueous Solubility Prediction Method
tf	161.00	K	KDB
tf	160.75 ± 0.30	K	NIST Webbook
tc	569.50	K	KDB
tc	577.50	K	NIST Webbook
tb	374.80	K	KDB
sl	327.02	J/mol×K	NIST Webbook
ripol	955.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	948.00		NIST Webbook
ripol	948.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.39	J/mol×K	511.68	Joback Method
cpg	169.62	J/mol×K	542.61	Joback Method
cpg	127.53	J/mol×K	357.08	Joback Method
cpg	135.38	J/mol×K	388.00	Joback Method
cpg	142.88	J/mol×K	418.92	Joback Method
cpg	150.04	J/mol×K	449.84	Joback Method
cpg	156.87	J/mol×K	480.76	Joback Method
cpl	173.26	J/mol × K	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

cpl	164.22	J/mol×K	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	164.78	J/mol×K	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	165.34	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	165.94	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	166.49	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	167.09	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	162.20	J/mol×K	298.15	NIST Webbook	
cpl	167.67	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	168.29	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	168.83	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	169.45	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	170.09	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	170.63	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	163.08	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	159.45	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	159.98	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	160.53	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	161.01	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	161.52	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	171.00	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	171.94	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	172.57	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	152.21	J/mol×K	292.30	NIST Webbook	
cpl	151.00	J/mol×K	298.00	NIST Webbook	
cpl	163.72	J/mol×K	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	175.47	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	175.19	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	174.51	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	162.08	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	173.89	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	162.60	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	
dvisc	0.0005750	Paxs	303.15	Densities and Viscosities of Binary Mixtures of 1-Bromobutane with Butanol Isomers at Several Temperatures	

dvisc	0.0006770	Paxs	288.15	Densities and Viscosities of Binary Mixtures of 1-Bromobutane with Butanol Isomers at Several Temperatures
dvisc	0.0006070	Paxs	298.15	Densities and Viscosities of Binary Mixtures
				of 1-Bromobutane with Butanol Isomers at Several Temperatures
dvisc	0.0005500	Paxs	308.15	Densities and Viscosities of Binary and Ternary Mixtures of (Nitrobenzene + 1-Bromobutane), (1-Bromobutane + Methylcyclohexane),
				(Nitrobenzene + Methylcyclohexane), and (Methylcyclohexane + Nitrobenzene + 1-Bromobutane) from (293.15 to 308.15) K
dvisc	0.0005811	Paxs	303.15	Densities and Viscosities of Binary and Ternary Mixtures of (Nitrobenzene
				1-Bromobutane), (1-Bromobutane + Methylcyclohexane), (Nitrobenzene + Methylcyclohexane),
				and (Methylcyclohexane + Nitrobenzene + 1-Bromobutane) from (293.15 to 308.15) K

dvisc	0.0006096	Paxs	298.15	Densities and Viscosities of Binary and Ternary Mixtures of (Nitrobenzene + 1-Bromobutane), (1-Bromobutane + Methylcyclohexane), (Nitrobenzene + Methylcyclohexane), and (Methylcyclohexane + Nitrobenzene + 1-Bromobutane) from (293.15 to 308.15) K	
dvisc	0.0006473	Paxs	293.15	Densities and Viscosities of Binary and Ternary Mixtures of (Nitrobenzene + 1-Bromobutane), (1-Bromobutane + Methylcyclohexane), (Nitrobenzene + Methylcyclohexane), and (Methylcyclohexane + Nitrobenzene + 1-Bromobutane) from (293.15 to 308.15) K	
dvisc	0.0004940	Paxs	318.15	Densities and Viscosities of Binary Mixtures of 1-Bromobutane with Butanol Isomers at Several Temperatures	
dvisc	0.0005190	Paxs	313.15	Densities and Viscosities of Binary Mixtures of 1-Bromobutane with Butanol Isomers at Several Temperatures	
dvisc	0.0005460	Paxs	308.15	Densities and Viscosities of Binary Mixtures of 1-Bromobutane with Butanol Isomers at Several Temperatures	
hfust	9.23	kJ/mol	160.40	NIST Webbook	
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hfust	9.23	kJ/mol	160.40	NIST Webbook	
hfust	9.23	kJ/mol	160.40	NIST Webbook	
hvapt	34.50 ± 0.10	kJ/mol	339.00	NIST Webbook	
hvapt	32.60	kJ/mol	372.40	NIST Webbook	
hvapt	33.00 ± 0.10	kJ/mol	366.00	NIST Webbook	
hvapt	33.50	kJ/mol	318.00	NIST Webbook	
hvapt	34.90 ± 0.10	kJ/mol	332.00	NIST Webbook	
hvapt	35.60 ± 0.10	kJ/mol	322.00	NIST Webbook	
hvapt	37.50	kJ/mol	336.50	NIST Webbook	
hvapt	34.60	kJ/mol	355.50	NIST Webbook	
hvapt	32.51	kJ/mol	374.70	NIST Webbook	
hvapt	33.70 ± 0.10	kJ/mol	352.00	NIST Webbook	
hvapt	36.77	kJ/mol	374.80	KDB	
pvap	8.90	kPa	308.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol	
pvap	1.86	kPa	278.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol	
pvap	2.48	kPa	283.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol	
pvap	3.27	kPa	288.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol	

pvap	4.26	kPa	293.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
pvap	5.51	kPa	298.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
pvap	7.04	kPa	303.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
pvap	13.87	kPa	318.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol
pvap	11.15	kPa	313.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol
pvap	8.90	kPa	308.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol

pvap	7.04	kPa	303.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol	
pvap	5.51	kPa	298.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol	
pvap	4.26	kPa	293.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol	
pvap	3.27	kPa	288.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol	
pvap	2.48	kPa	283.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol	
pvap	1.86	kPa	278.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol	

pvap	17.09	kPa	323.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
pvap	13.87	kPa	318.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
pvap	17.09	kPa	323.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T) 298.15 K for 1-Bromobutane with 1-Octanol or 1-Decanol
pvap	11.15	kPa	313.15	Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at T = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
rhol	1229.50	kg/m3	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1313.80	kg/m3	263.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1300.50	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rhol	1286.40	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1265.70	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1326.50	kg/m3	253.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
sfust	57.57	J/mol×K	160.40	NIST Webbook
sfust	57.57	J/mol×K	160.40	NIST Webbook
speedsl	735.21	m/s	383.31	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	797.60	m/s	363.23	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	861.16	m/s	343.22	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	925.99	m/s	323.22	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	1090.98	m/s	273.26	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	
speedsl	1195.27	m/s	243.38	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	

Correlations

Information Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47590e+01
Coeff. B	-3.37027e+03
Coeff. C	-4.16480e+01
Temperature range (K), min.	274.54
Temperature range (K), max.	398.38

Information Value

Property code	pvap
Equation	$ln(Pvp) = A + B/T + C*ln(T) + D*T^2$
Coeff. A	1.18191e+02
Coeff. B	-8.35117e+03
Coeff. C	-1.57561e+01
Coeff. D	1.48094e-05
Temperature range (K), min.	160.75
Temperature range (K), max.	577.00

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Vapor Liquid Equilibrium between https://www.doi.org/10.1021/je020110g Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Pensitions and Visuositions of John Mitter and Visuositions and Tanana Mitter and Visuositions of John Mitter and Visuositions of Liquid Microwall Material Compressibilities of Liquid Microwall Material Research Temperatures from (243.15 to 423.15) K:

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

https://www.cheric.org/files/research/kdb/mol/mol1606.mol

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

(243.15 to 423.15) K. The Yaws Handbook of Vapor https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Pressure: Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method:

Density of Some 1-Bromoalkanes https://www.doi.org/10.1021/je700015t

https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1606

within the Temperature Range from [A28 Byre (A29 Parametrics Databank):
Heat Capacities of 1-chloroalkanes and https://www.doi.org/10.1021/je049652j 1-bromoalkanes within the temperature Tangendynasyics of lovest-implication A Breggradsiji Bramphytanaland Its Galhernity analysis. https://www.doi.org/10.1021/je200814m

https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1606

Densities and Viscosities of Binary https://www.doi.org/10.1021/je0501235

Mixtures of 1-Bromobutane with http://webbook.nist.gov/cgi/cbook.cgi?ID=C109659&Units=SI Temperatures:

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

Ideal gas heat capacity cpg: Liquid phase heat capacity cpl:

dvisc: Dynamic viscosity

Standard Gibbs free energy of formation gf: 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 Octanol/Water partition coefficient logp: mcvol: McGowan's characteristic volume

Critical Pressure pc: Vapor pressure pvap: rhol: 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

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

zc: Critical Compressibility

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