

Butanal

Other names:	1-Butanal 1-propanecarbaldehyde Aldehyde butyrique Aldeide butirrica BUTAL BUTYL ALDEHYDE Butaldehyde Butalyde Butan-1-al Butanaldehyde Butyral Butyraldehyd Butyraldehyde Butyric aldehyde Butyrylaldehyde NCI-C56291 NSC 62779 UN 1129 n-Butanal n-Butyl aldehyde n-Butyraldehyde n-C3H7CHO propanecarbaldehyde
Inchi:	InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3
InchiKey:	ZTQSAGDEMFDKMZ-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	CCCC=O
Mol. weight [g/mol]:	72.11
CAS:	123-72-8

Physical Properties

Property code	Value	Unit	Source
af	0.3520		KDB
affp	792.70	kJ/mol	NIST Webbook
aigt	503.15	K	KDB
basg	760.80	kJ/mol	NIST Webbook

chl	-2478.70 ± 0.71	kJ/mol	NIST Webbook
chl	-2477.10 ± 1.40	kJ/mol	NIST Webbook
dm	2.60	debye	KDB
ea	6.94e-04	eV	NIST Webbook
fll	2.50	% in Air	KDB
flu	10.60	% in Air	KDB
fpc	263.71	K	KDB
fpo	266.48	K	KDB
gf	-114.80	kJ/mol	KDB
hf	-204.40 ± 1.40	kJ/mol	NIST Webbook
hf	-206.70	kJ/mol	NIST Webbook
hf	-211.80 ± 0.92	kJ/mol	NIST Webbook
hf	-205.10	kJ/mol	NIST Webbook
hf	-205.20	kJ/mol	KDB
hfl	-238.10 ± 1.50	kJ/mol	NIST Webbook
hfl	-245.40 ± 0.84	kJ/mol	NIST Webbook
hfl	-238.70 ± 0.71	kJ/mol	NIST Webbook
hfl	-240.30	kJ/mol	NIST Webbook
hfus	8.40	kJ/mol	Joback Method
hvap	33.20	kJ/mol	NIST Webbook
hvap	33.70 ± 0.40	kJ/mol	NIST Webbook
hvap	33.60	kJ/mol	NIST Webbook
hvap	33.70	kJ/mol	NIST Webbook
hvap	33.70 ± 0.40	kJ/mol	NIST Webbook
ie	9.73 ± 0.03	eV	NIST Webbook
ie	9.83	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.82 ± 0.04	eV	NIST Webbook
ie	9.83	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.86 ± 0.02	eV	NIST Webbook
ie	9.84 ± 0.01	eV	NIST Webbook
ie	9.73 ± 0.01	eV	NIST Webbook
log10ws	-1.00e-02		Aqueous Solubility Prediction Method
log10ws	-0.01		Estimated Solubility Method
logp	0.985		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	4320.00 ± 100.00	kPa	NIST Webbook
pc	4320.00	kPa	KDB
rhoc	279.77 ± 5.05	kg/m3	NIST Webbook

rinpol	554.00	NIST Webbook
rinpol	580.49	NIST Webbook
rinpol	583.70	NIST Webbook
rinpol	587.66	NIST Webbook
rinpol	588.95	NIST Webbook
rinpol	615.44	NIST Webbook
rinpol	618.79	NIST Webbook
rinpol	573.33	NIST Webbook
rinpol	570.90	NIST Webbook
rinpol	570.70	NIST Webbook
rinpol	571.10	NIST Webbook
rinpol	571.90	NIST Webbook
rinpol	572.54	NIST Webbook
rinpol	542.10	NIST Webbook
rinpol	573.00	NIST Webbook
rinpol	571.00	NIST Webbook
rinpol	572.00	NIST Webbook
rinpol	572.00	NIST Webbook
rinpol	574.00	NIST Webbook
rinpol	574.00	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	563.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	578.18	NIST Webbook
rinpol	568.00	NIST Webbook
rinpol	555.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	586.00	NIST Webbook
rinpol	586.00	NIST Webbook
rinpol	605.00	NIST Webbook
rinpol	594.00	NIST Webbook
rinpol	593.00	NIST Webbook
rinpol	600.00	NIST Webbook
rinpol	561.00	NIST Webbook
rinpol	589.50	NIST Webbook
rinpol	593.00	NIST Webbook
rinpol	600.00	NIST Webbook
rinpol	575.00	NIST Webbook
rinpol	571.00	NIST Webbook
rinpol	570.00	NIST Webbook
rinpol	613.00	NIST Webbook
rinpol	598.00	NIST Webbook
rinpol	596.00	NIST Webbook
rinpol	595.00	NIST Webbook

rinpol	596.00	NIST Webbook
rinpol	571.00	NIST Webbook
rinpol	562.00	NIST Webbook
rinpol	545.00	NIST Webbook
rinpol	593.00	NIST Webbook
rinpol	598.00	NIST Webbook
rinpol	601.00	NIST Webbook
rinpol	593.00	NIST Webbook
rinpol	563.31	NIST Webbook
rinpol	595.00	NIST Webbook
rinpol	596.00	NIST Webbook
rinpol	596.00	NIST Webbook
rinpol	587.00	NIST Webbook
rinpol	564.00	NIST Webbook
rinpol	565.00	NIST Webbook
rinpol	576.00	NIST Webbook
rinpol	583.00	NIST Webbook
rinpol	582.00	NIST Webbook
rinpol	614.00	NIST Webbook
rinpol	572.00	NIST Webbook
rinpol	591.00	NIST Webbook
rinpol	571.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	571.00	NIST Webbook
rinpol	593.00	NIST Webbook
rinpol	564.00	NIST Webbook
rinpol	607.00	NIST Webbook
rinpol	568.00	NIST Webbook
rinpol	563.00	NIST Webbook
rinpol	563.00	NIST Webbook
rinpol	568.00	NIST Webbook
rinpol	575.99	NIST Webbook
rinpol	575.00	NIST Webbook
rinpol	574.00	NIST Webbook
rinpol	571.50	NIST Webbook
rinpol	573.77	NIST Webbook
rinpol	587.66	NIST Webbook
rinpol	570.90	NIST Webbook
rinpol	542.10	NIST Webbook
rinpol	573.77	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	586.00	NIST Webbook
rinpol	605.00	NIST Webbook
rinpol	571.57	NIST Webbook

ripol	569.15	NIST Webbook
ripol	568.78	NIST Webbook
ripol	570.91	NIST Webbook
ripol	571.50	NIST Webbook
ripol	589.00	NIST Webbook
ripol	574.00	NIST Webbook
ripol	899.00	NIST Webbook
ripol	853.00	NIST Webbook
ripol	877.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	891.00	NIST Webbook
ripol	910.00	NIST Webbook
ripol	898.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	875.00	NIST Webbook
ripol	885.00	NIST Webbook
ripol	832.00	NIST Webbook
ripol	865.00	NIST Webbook
ripol	877.00	NIST Webbook
ripol	895.00	NIST Webbook
ripol	837.00	NIST Webbook
ripol	867.00	NIST Webbook
ripol	859.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	878.00	NIST Webbook
ripol	861.00	NIST Webbook
ripol	861.00	NIST Webbook
ripol	891.00	NIST Webbook
ripol	875.00	NIST Webbook
ripol	864.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	877.00	NIST Webbook
ripol	839.00	NIST Webbook
ripol	839.00	NIST Webbook
ripol	839.00	NIST Webbook
ripol	867.00	NIST Webbook
ripol	886.00	NIST Webbook
ripol	895.00	NIST Webbook
ripol	895.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	905.00	NIST Webbook
ripol	854.46	NIST Webbook
ripol	867.47	NIST Webbook
ripol	874.62	NIST Webbook

ripol	891.30		NIST Webbook
ripol	911.46		NIST Webbook
ripol	907.20		NIST Webbook
ripol	894.80		NIST Webbook
ripol	897.80		NIST Webbook
ripol	901.80		NIST Webbook
ripol	906.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	853.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	877.00		NIST Webbook
ripol	899.00		NIST Webbook
ripol	891.00		NIST Webbook
ripol	877.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	881.00		NIST Webbook
ripol	830.00		NIST Webbook
ripol	831.00		NIST Webbook
ripol	862.00		NIST Webbook
ripol	887.00		NIST Webbook
ripol	878.00		NIST Webbook
ripol	895.00		NIST Webbook
ripol	866.00		NIST Webbook
sg	344.80 ± 4.20	J/molxK	NIST Webbook
sl	246.90	J/molxK	NIST Webbook
sl	242.70	J/molxK	NIST Webbook
tb	348.15 ± 3.00	K	NIST Webbook
tb	347.94 ± 0.30	K	NIST Webbook
tb	348.15 ± 2.00	K	NIST Webbook
tb	347.95 ± 0.40	K	NIST Webbook
tb	346.65 ± 2.00	K	NIST Webbook
tb	348.15 ± 2.00	K	NIST Webbook
tb	345.65 ± 3.00	K	NIST Webbook
tb	348.15 ± 2.00	K	NIST Webbook

tb	75.70 ± 0.50	K	NIST Webbook
tb	347.40 ± 1.00	K	NIST Webbook
tb	350.15 ± 1.00	K	NIST Webbook
tb	346.00 ± 3.00	K	NIST Webbook
tb	1021.99 ± 0.10	K	NIST Webbook
tb	347.85 ± 0.50	K	NIST Webbook
tb	346.65 ± 2.00	K	NIST Webbook
tb	346.65 ± 1.00	K	NIST Webbook
tb	348.05 ± 1.00	K	NIST Webbook
tb	346.15 ± 2.00	K	NIST Webbook
tb	347.95 ± 0.30	K	NIST Webbook
tb	347.75 ± 0.50	K	NIST Webbook
tb	348.65 ± 1.00	K	NIST Webbook
tb	347.95	K	NIST Webbook
tb	348.65 ± 1.00	K	NIST Webbook
tb	348.35 ± 0.50	K	NIST Webbook
tb	346.00 ± 3.00	K	NIST Webbook
tb	348.40 ± 0.60	K	NIST Webbook
tb	348.35 ± 0.50	K	NIST Webbook
tb	347.35 ± 1.00	K	NIST Webbook
tb	344.90 ± 3.00	K	NIST Webbook
tb	347.85 ± 1.00	K	NIST Webbook
tb	347.65 ± 0.50	K	NIST Webbook
tb	347.40 ± 0.50	K	NIST Webbook
tb	349.15 ± 2.00	K	NIST Webbook
tb	347.90	K	KDB
tb	348.70	K	NIST Webbook
tc	537.10 ± 4.00	K	NIST Webbook
tc	537.20	K	KDB
tc	537.20 ± 0.80	K	NIST Webbook
tf	175.40	K	Aqueous Solubility Prediction Method
tf	174.00	K	KDB
tt	176.28 ± 0.02	K	NIST Webbook
tt	176.80 ± 0.20	K	NIST Webbook
tt	176.80 ± 0.20	K	NIST Webbook
vc	0.258	m ³ /kmol	KDB
zc	0.2495350		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	119.02	J/molxK	368.40	Joback Method
cpg	138.22	J/molxK	454.86	Joback Method
cpg	132.06	J/molxK	426.04	Joback Method
cpg	149.84	J/molxK	512.50	Joback Method
cpg	112.13	J/molxK	339.58	Joback Method
cpg	125.66	J/molxK	397.22	Joback Method
cpg	144.14	J/molxK	483.68	Joback Method
cpl	164.70	J/molxK	298.15	NIST Webbook
cpl	163.51	J/molxK	298.15	NIST Webbook
dvisc	0.0003900	Paxs	308.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
dvisc	0.0004000	Paxs	303.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
dvisc	0.0003600	Paxs	313.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
dvisc	0.0003500	Paxs	318.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures

dvisc	0.0003200	Paxs	323.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
dvisc	0.0004300	Paxs	298.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
hfust	10.77	kJ/mol	176.28	NIST Webbook
hfust	11.10	kJ/mol	176.80	NIST Webbook
hfust	11.09	kJ/mol	176.80	NIST Webbook
hvapt	31.51	kJ/mol	347.90	KDB
hvapt	33.90	kJ/mol	305.50	NIST Webbook
hvapt	33.30	kJ/mol	325.50	NIST Webbook
hvapt	32.90	kJ/mol	339.00	NIST Webbook
hvapt	34.20	kJ/mol	321.00	NIST Webbook
rfi	1.38390		293.15	Liquid Liquid Equilibrium Data of Water + Butyric Acid + {Butanal or n-Butanol} Ternary Systems at 293.15, 308.15, and 323.15 K
rhoI	802.00	kg/m3	293.00	KDB
rhoI	771.30	kg/m3	323.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures

rho1	781.37	kg/m3	313.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
rho1	786.41	kg/m3	308.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
rho1	791.80	kg/m3	303.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
rho1	796.99	kg/m3	298.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
rho1	801.54	kg/m3	293.15	Liquid Liquid Equilibrium Data of Water + Butyric Acid + {Butanal or n-Butanol} Ternary Systems at 293.15, 308.15, and 323.15 K

rhoI	776.39	kg/m ³	318.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
sfust	61.11	J/mol×K	176.28	NIST Webbook
sfust	62.81	J/mol×K	176.80	NIST Webbook
speedsl	1193.85	m/s	298.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
speedsl	1088.76	m/s	323.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
speedsl	1109.64	m/s	318.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
speedsl	1130.57	m/s	313.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures

speedsl	1151.60	m/s	308.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
speedsl	1172.70	m/s	303.15	Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures
srf	0.02	N/m	293.20	KDB

Sources

Binary mixtures of ([C4mim][NTf2] + molecular organic solvents): Thermophysical, acoustic and transport properties at various compositions and temperatures: KDB

<https://www.doi.org/10.1016/j.jct.2015.09.022>

Aqueous Solubility Prediction Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C123728&Units=SI>

Estimated Solubility Method:

<https://www.chemic.org/files/research/kdb/mol/mol1234.mol>

Crippen Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method:

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

Liquid Liquid Equilibrium Data of Water + Butyric Acid + {Butanal or n-Butanol} Ternary Systems at 293.15, 308.15, and 323.15 K:

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

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

<https://www.doi.org/10.1021/acs.jced.6b00941>

Joback Method:

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

Legend

af:	Acentric Factor
affp:	Proton affinity
aight:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity

cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
fill:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
rfi:	Refractive Index
rhoc:	Critical density
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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