

® = Registered trademark of BASF SE

n-BUTANOL

Colourless, mobile solvent of medium volatility. Feedstock for syntheses.

Chemical nature

n-butanol, n-butyl alcohol, 1-butanol

 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$

Molecular formula: $\text{C}_4\text{H}_{10}\text{O}$

Molar mass: 74.12 g/mol

CAS-Number: 71-36-3

EC-Number: 200-751-6

Delivery specification

Property	Value	Unit	Test method
Mass fraction of			
– n-butanol	99.8 min.	%	DIN 55685
– isobutanol	0.1 max.	%	
– butyl ether	0.02 max.	%	
– butyraldehyde	0.05 max.	%	
– water	0.05 max.	%	DIN 51777, Part 1
Pt/Co-colour	5 max.		DIN EN ISO 6271
Acid value	0.03 max.	mg/KOH/g	DIN EN ISO 2114
Acidity	0.003 max.	%	calculated as acetic acid

Properties

n-Butanol is a clear, mobile, neutral liquid with a characteristic odour. It is miscible with all common solvents, e. g. alcohols, ketones, aldehydes, ethers, glycols, and aromatic and aliphatic hydrocarbons. Its miscibility with water, however, is restricted.

The product conforms to the specifications laid down in DIN 53245.

Physical data

The following physical data have been compiled from the literature as well as from BASF measurements and calculations. They provide no guarantee of properties in the legal sense, however.

Boiling range at 1013 hPa 116–118 °C
(DIN 53171; 95 Vol.-%; 2–97 ml)

Density at 20 °C (DIN 51757) 0.809–0.811 g/cm³

Refractive index n_D^{20} (DIN 53491) 1.398–1.400

Solidification point at 1013 hPa –89.3 °C

T [°C]	Density ρ [g/cm ³]	Viscosity η [mPa · s]	Surface tension σ [mN/m]	Refractive index n_D	Dielectric constant ϵ
–50	0.8518	34.5			
–30	0.8414	14.8			
0	0.8233	5.2	26.3	1.4073	20.6
10	0.8166	3.9	25.5	1.4033	19.1
20	0.8096	2.9	24.7	1.3992	17.7
30	0.8022	2.3	23.9	1.3950	16.5
40	0.7946	1.8	23.0	1.3908	15.4
50	0.7866	1.4	22.2	1.3865	14.4
60	0.7783	1.1			
80	0.7608	0.8			
100	0.7419	0.5			

T [°C]	Specific heat C_p [kJ/(kg · K)]	Thermal conductivity λ [mW/(m · K)]	Vapour pressure P (hPa)
0	2.264	170.0	0.96
10	2.318	168.5	2.4
20	2.372	167.0	5.6
30	2.426	165.6	11.9
40	2.480	164.4	23.7
50	2.534	163.2	44.3
60	2.589	162.2	78.7
80	2.698	160.4	217.0
100	2.808	159.0	517.9
110			764.5
117.7			1013

Heat of combustion (ΔH_c) 36111 kJ/Kg

Heat of vaporisation (ΔH_v) 592 kJ/kg

Heat of fusion 125 kJ/kg

Evaporation rate (DIN 53170; ether = 1) 33

Solubility**Mass fraction of**

– n-Butanol in water	at 20 °C	7.7 %
	at 30 °C	7.1 %
– water in n-Butanol	at 20 °C	20.1 %
	at 30 °C	20.6 %

Hansen solubility parameter at 25 °C:

$$\delta_d = 16.0 \text{ (MPa)}^{1/2}$$

$$\delta_p = 5.7 \text{ (MPa)}^{1/2}$$

$$\delta_h = 15.8 \text{ (MPa)}^{1/2}$$

$$\delta_t = 23.1 \text{ (MPa)}^{1/2}$$

$$\text{Conversion factor: } 1 \text{ (cal/cm}^3)^{1/2} = 2,0455 \text{ (MPa)}^{1/2}$$

Applications

n-Butanol is used as a solvent and as a feedstock for syntheses.

A survey of the various applications is presented below, but does not claim to be complete.

About half of the production of pure n-Butanol and its derivatives (primarily esters) is used as solvents in the coatings industry. The advantage here is that n-butanol prevents blushing of certain coatings when they dry under humid conditions. Thus it is widely used as a diluent in cellulose nitrate lacquers and serves to improve their flow, gloss and resistance to blushing (blushing only occurs in the presence of volatile solvents and at high humidities). For this purpose addition rates of 5–10 % are generally sufficient.

n-Butanol is an eminently suitable solvent for acid-curable lacquers and baking finishes derived from urea (Plastopal®), melamine (Luwipal®), or phenolic resins. In these applications, it is mostly used together with glycol ethers or ethanol.

When added even in small proportions to alkyd resin paints, n-Butanol reduces their viscosity and thus improves their brushability and flow. Low concentrations of n-Butanol prevent cobwebbing in lacquers formulated from spirit-soluble resins.

Some butyl esters of dicarboxylic acids, phthalic anhydride and acrylic acid are established plasticizers for plastics, rubber mixes and dispersions. The most important are dibutyl phthalate (DBP), benzylbutyl phthalate (BBP) and butyl acrylate. Dibutyl sebacate (DBS) and dibutyl azelate (DBZ) are of lesser importance. The corresponding adipate is too volatile as a plasticizer and therefore of no practical significance in these applications.

Other applications for n-Butanol are as follows.

- Solvent for dyes, e. g. in printing inks.
- Extractant in the production of drugs and natural substances such as antibiotics, hormones, vitamins, alkaloids and camphor.
- Additive in polishes and cleaners, e. g. floor cleaners and stain removers.
- Solubilizer in the textile industry, e. g. additive in spinning baths or carrier for colouring plastics.
- Additive in de-icing fluids.
- Additive in gasoline for spark-ignition engines (prevents carburettor icing).
- Mobile phase in paper and thin-layer chromatography.
- Humectant for cellulose nitrate.
- Feedstock for the production of glycol ethers (in reaction with ethylene or propylene oxide).
- Starting material for various butyl monocarboxylates, e. g. butyl acetate and butyl butyrate, which are widely used as solvents.
- Feedstock for the production of flotation aids, e. g. butyl xanthate.

The butyl esters of various dicarboxylic acids, e.g. sebacic, adipic and stearic acids, are used as synthetic and semisynthetic lubricants and hydraulic fluids.

Storage

n-Butanol can be stored in suitable containers at temperatures below 40 °C and the exclusion of humidity for at least 1 year.

Safety

When using this product, the information and advice given in our **Safety Data Sheet** should be observed. Due attention should also be given to the **precautions** necessary for handling chemicals.

Note

The data contained in this publication are based on our current knowledge and experience. In view of the many factors that may affect processing and application of our product, these data do not relieve processors from carrying out their own investigations and tests; neither do these data imply any guarantee of certain properties, nor the suitability of the product for a specific purpose. Any descriptions, drawings, photographs, data, proportions, weights etc. given herein may change without prior information and do not constitute the agreed contractual quality of the product. It is the responsibility of the recipient of our products to ensure that any proprietary rights and existing laws and legislation are observed.

March 2008