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ISOBUTANOL

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

Chemical nature

Isobutanol, isobutyl alcohol, 2-methyl-1-propanol

Molecular formula: C₄ H₁₀ O

Molar mass: 74.12 g/mol

CAS- Number: 78-83-1

EC- Number: 201-148-0

Delivery specification

Property	Value	Unit	Test method DIN/ASTM
Mass fraction of – isobutanol	99.5 min.	%	55685/GC
– water	0.05 max.	%	51777, part 1/D 1364
Platinum-cobalt colour	5 max.	–	ISO 6271/D 1209
Acidity [1] (as acetic acid)	0.003 max.	%	EN ISO 2114/D 1613
[1] Acid number	max. 0.03	mg KOH/g	

Properties

Isobutanol 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 limited.

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 mbar (DIN 53171; 95 Vol.-%; 2 – 97 ml)	106 – 108 °C
Density at 20 °C (DIN 51757)	0.801 – 0.803 g/cm ³
Refractive index n_D^{20} (DIN 51757)	1.395 – 1.396
Solidification point at 1013 mbar	–108 °C

T [°C]	Vapour Pressure [mbar]	Density ρ [g/cm ³]	Viscosity η [mPa · s]	Refractive Index n_D
– 30	0.05	0.8361		1.4136
– 20	0.2	0.8302	18.4	1.4103
– 10	0.6	0.8238		1.4069
0	1.7	0.8171	8.3	1.4033
10	4.2	0.8100		1.3996
20	9.5	0.8025	3.95	1.3957
30	19.8			
40	38.6	0.7863	2.12	1.3875
50	70.7	0.7778		1.3832
60	123	0.7684	1.24	1.3787
80	327	0.7490	0.78	1.3694
100	753	0.7279	0.52	1.3595
107.9	1013			

T [°C]	Specific heat C_p [kJ/(kg · K)]	Thermal conductivity λ [mW/(m · K)]
0	1.909	137.0
10	2.102	135.2
20	2.303	133.3
30	2.508	131.5
40	2.713	129.6
50	2.914	127.8
60	3.106	125.9

Heat of combustion (ΔH_c)	at 25 °C*	36 023 kJ/kg
Enthalpy of vaporization (ΔH_v)	at 25 °C*	579 kJ/kg
Enthalpy of formation (ΔH_f)	at 25 °C*	4509 kJ/kg
Surface tension	at 20 °C at 30 °C	23.0 mN/m 22.1 mN/m
Dielectric constant	at 0 °C at 30 °C	21.1 17.3
Evaporation rate (DIN 5310; ether = 1)		25

Solubility

Mass fraction of		
– isobutanol in water	at 20 °C	8.5 %
	at 30 °C	7.5 %
– water in isobutanol	at 20 °C	15.0 %
	at 30 °C	17.3 %

*) *calculated*

Hansen solubility parameters at 25 °C:

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

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

$$\delta_h = 14.5 \text{ (MPa)}^{1/2}$$

$$\delta_t = 22.2 \text{ (MPa)}^{1/2}$$

Applications

Isobutanol 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.

A major part of the production of pure Isobutanol is converted into derivatives (primarily esters) which are used as solvents in the coating industry. The advantage here is that Isobutanol 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.

Isobutanol is an eminently suitable solvent for acid-curable lacquers and baking finishes derived from urea (Plastopal®), melamine (Luwipal®), or phenolic resins. Here it is mainly used together with glycol ethers, ethanol or aromatic hydrocarbons.

Even when added in small proportions to alkyd resin paints, Isobutanol reduces their viscosity and thus improves their brushability and flow. Low concentrations of Isobutanol prevent cobwebbing in lacquers formulated from spirit-soluble resins and exert a beneficial effect in water-based paints.

Di-isobutyl phthalate (DIBP) has gained importance amongst the isobutyl esters of dicarboxylic acids as a plasticizer for plastics, dispersions and rubber mixes. Other isobutyl esters of dicarboxylic acids, e. g. adipic, azelaic and sebacic acids, display good properties in this application. Economic considerations, however, preclude their use at present.

Other applications for Isobutanol are as follows:

- Solvent for 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.
- Dehydrating agent (entrainer in azeotropic distillation).
- Feedstock in the production of glycol ethers (in reactions with ethylene or propylene oxides).
- Feedstock in the production of flotation aids (e. g. isobutyl xanthate).
- Starting material in the production of wear inhibitors and anticorrosion additives in engine oils, e. g. zinc diisobutyl dithiophosphate.

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

Storage

Isobutanol can be stored in suitable containers at temperature below 40 ° 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.

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