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2-ETHYLHEXANOL

High-boiling point, low-volatility solvent for fats, waxes, dyes and insecticides. Starting material for the manufacture of plasticizers, lubricants and other chemical products such as raw materials for paints and coatings.

Chemical nature

2-Ethylhexan-1-ol
2-Ethyl-1-hexanol;
Isooctanol

Molecular formula: C₈H₁₈O
Molar mass: 130.23 g/mol
CAS-No.: 104-76-7 EINECS-No.: 203-234-3

Delivery specification

Property	Value	Unit	Test method
Mass fraction			
- 2-ethylhexanol	min. 99.5	%	gas chromatography, BASF method
- water (on despatch)	max. 0.05	%	DIN 51777, part 1
Platinum-cobalt colour	max. 10	-	DIN ISO 6271

General information can be found in [1].

Properties

2-ethylhexanol is a clear, mobile and neutral liquid with a characteristic odour. It is miscible with most common organic solvents but its miscibility with water is very limited.

2-ethylhexanol enters into the reactions that are typical of primary alcohols. For instance, it readily forms esters with various acids.

Chemicals

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)	183 -185 °C
Density at 20 °C (DIN 51757)	0.832 - 0.834 g/cm ³
Refractive index n _D ²⁰ (DIN 53491)	1.431 -1.432
Refractive index n _D ⁴⁰	1.4237
Freezing point (at 1013 mbar)	- 76 °C (glass trans. temperature)

T [°C]	Vapour pressure p [mbar]	Density ρ [g/cm ³]	Viscosity η [mPa · s]	Surface Tension σ [mN/m]
-10	0.002			
0	0.01	0.8476	17.7	25.1
10	0.04	0.8401	12.2	24.2
20	0.14	0.8326	8.8	23.2
40	0.8	0.8178	5.1	21.4
50	1.8			
60	3.9	0.8031	3.2	19.6
80	14.4	0.7886	2.1	17.8
100	43.0	0.7743	1.4	16.1
120	109			
140	243			
160	487			
180	897			
184.3	1013			

T [°C]	Specific heat capacity of the liquid C _{p fl.} [kJ/(kg · K)]	Specific heat capacity of the gas C _{p g.} [kJ/(kg · K)]	Thermal conductivity λ [mW/(m · K)]
0	2.36	1.42	41.2
10	2.38	1.46	70.8
20	2.41	1.51	95.8
40	2.45	1.60	133.8
60	2.50	1.69	158.8
80	2.55	1.77	174.5
100	2.60	1.85	184.3
120	2.64	1.93	191.8
140	2.68	2.01	200.7

Heat of combustion (ΔH _c) at 25 °C*	38 044 kJ/kg
Heat of formation (ΔH _f)	- 3 326 kJ/kg
Enthalpy of vaporization (ΔH _v) bei 1013 mbar	358 kJ/kg
Dipolar moment (μ)	1.8 D
Dielectric constant at 90 °C	4.41

Evaporation rate (DIN 53170; ether = 1)

approx. 600

Solubility parameter at 25 °C according to Hansen:

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

$$\text{TM}_p = 3.3 \text{ (MPa)}^{1/2}$$

$$\text{TM}_h = 11.9 \text{ (MPa)}^{1/2}$$

$$\text{TM}_t = 20.2 \text{ (MPa)}^{1/2}$$

*) *calculated*

Applications

2-Ethylhexanol is not widely used as a solvent. Its main application is as a feedstock in the manufacture of low-volatility esters, the most important of which is di-(2-ethylhexyl) phthalate (DOP, DEHP, Palatinol ® AH), which is an all-purpose plasticizer for PVC and vinyl chloride copolymers. The features of this plasticizer are its low volatility, excellent gelling power, its great resistance to high and low temperatures and to water, and its outstanding dielectric properties.

Other plasticizers that can be used to obtain specific properties are the corresponding esters of 2-ethylhexanol and

- adipic acid (e. g. Plastomoll → DOA)
- para-hydroxybenzoic acid
- sebacic acid
- azelaic acid
- trimellitic acid
- stearic acid
- terephthalic acid
- phosphoric acid, etc.

Additionally, phthalate plasticizers can be obtained from mixtures of 2-ethylhexanol and other alcohols.

Examples of other applications for 2-ethylhexanol are summarized below. The list is by no means complete.

- Low-volatility solvent (e. g. for resins, waxes, animal fats, vegetable oils and petroleum derivatives).
- Low-volatility ingredient in solvent blends for the dyestuffs and coatings industry.
- Flow and gloss improver in baking finishes.
- Feedstock for the manufacture of ethoxylates (products of reaction between 2-ethylhexanol and ethylene oxide).
- Feedstock in the manufacture of herbicides.
- Feedstock in the manufacture of extractants (e.g. for heavy metals).
- In the production of the corresponding diester of maleic acid for use as a starting material for surfactants.
- Feedstock in the manufacture of 2-ethylhexyl sulphate which is used as a surfactant for electrolytes.
- In the production of 2-ethylhexyl esters of trialkyl phosphites which can serve as a thermal stabilizer and antioxidant in plastics.
- In the manufacture of particularly pure grades of DOP which act as polychlorinated biphenyl substitutes in heavy-duty capacitors.
- In antifoams for almost all aqueous systems (e. g. in the textile and paper industries)

Literature

[1] Technical Information Leaflet of BASF AG: "Gas-chromatographic determination of the degree of purity of solvents and plasticizers (a review)" (TI-CIW/ES 001 e).

Safety Data Sheet

A Safety Data Sheet according to EU guideline 91/155/EWG is available for 2-Ethylhexanol.

Note

The information submitted in this publication is based on our current knowledge and experience. In view of the many factors that may affect processing and application, these data do not relieve processors of the responsibility of carrying out their own tests and experiments; neither do they imply any legally binding assurance of certain properties or of suitability for a specific purpose. It is the responsibility of those to whom we supply our products to ensure that any proprietary rights and existing laws and legislation are observed.

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