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Propylheptanol

Alcohol as raw material for the production of plasticizers and auxiliaries in the chemical and allied industries.

Chemical nature

2-Propyl-1-heptanol, 2-propylheptane-1-ol,

Molecular formula	$C_{10}H_{22}O$
Molar mass	158.3 g/mol
CAS number	10042-59-8
EC-number	233-126-1

Delivery specification

Property	Value	Unit	Test method DIN/ASTM
Fraction of – decanol isomers	99.5 min.	% by area	by gaschromatography*
– water	0.1 max.	% by weight	DIN 51777, Part 1 E 203
Platinum-cobalt color	10 max.		DIN ISO 6271-2/ D 5386
Acid value	0.1 max.	mg KOH/g	DIN EN ISO 2114/ D 1045

* See page 3 for GC conditions

Properties

Propylheptanol is a clear, high-boiling liquid with a mild odor. It is miscible with most common organic solvents, but is practically insoluble in water.

Propylheptanol is a mixture of isomeric decyl alcohols and reacts accordingly. An example of an application of practical significance is the formation of the corresponding esters in reaction with acids.

Physical data

The following physical data were measured in the BASF SE laboratories. They do not represent any legally-binding guarantee of properties for our sales product.

Boiling range at 1013 hPa (96 % by vol.; 1–97 ml) 207 °C–212 °C (DIN 51751; ASTM D 1078)

Melting/crystallizing point <–50 °C (DIN 51007 BASF-modified)

Vapor pressure	T [°C]	p [hPa]
	20	0.02
	30	0.06
	40	0.14
	50	0.35
	60	0.8
	70	1.7
	80	3.4
	90	6.3
	100	11
	120	33
	140	80
	160	175
	180	346
	200	628
	220	1066

Equation for calculating the vapor pressure (T in Kelvin)

$$\ln(p/\text{Pa}) = 176.768 - 15780.6/T - 21.5291 \cdot \ln T + 2.12765E - 17 \cdot T^{**6}$$

(The equation constants were determined from vapor pressure data measured in the temperature range of 63 °C to 217 °C by a dynamic method in a nitrogen atmosphere. The values in the table were calculated using the equation. The data serve only as a rough guide.)

Density/viscosity	Temp. [°C]	Density* ρ [g/cm ³] (DIN 51757)	Dyn. viscosity** η [mPa · s] (DIN 51562)
	5	0.8425	33.7
	10	0.8391	25.5
	20	0.8322	15.2
	30	0.8253	9.7
	40	0.8182	6.5
	50	0.8111	4.5

* Calculated using the following equation: $\rho = (-0.0007T + 0.8461)$ from data measured by BASF SE.

(ρ = Density g/cm³, T = Temperature °C)

** Calculated: Kinematic viscosity (DIN 51562) multiplied with density.

Refractive index at 20 °C 1.4371

Surface tension at 20 °C (DIN EN 14370) 27.5 mN/m

Analytical data

Gas chromatography

The following conditions have been established in practice for the chromatographic assay:

Column:	Capillary column (fused silica WCOT) with CP-Sil-5-CB 25 m long, internal diameter 0.25 mm Film thickness: 0.12 µm
Temperatures:	Injector: 300 °C (splitting ratio approx. 1 : 150) Oven: 80 °C, then heated to 300 °C at 10 °C/min Detector: 300 °C
Carrier gas:	Nitrogen, high purity (approx. 1.5 ml/min)
Detector:	FID
Evaluation:	Area percent without correction factor

Applications

The main application for Propylheptanol is as a starting material for the production of plasticizers for PVC, e.g. Palatinol® 10-P.

Storage & Handling

Propylheptanol can be stored in tanks and drums constructed from normal carbon steel, e.g. A 283 grade. If severe demands are imposed on the product quality, we recommend that it be stored in tanks constructed from stainless steel, e.g. AISI TP 316 Ti (German steel No. 1.4541), or aluminium (AlMg₃).

It is recommended that steps be taken to ensure the exclusion of atmospheric moisture, e.g. by storing under a blanket of dry nitrogen, as otherwise the product quality may deteriorate, e.g. the water fraction may rise, or the Propylheptanol may be discolored by rust in normal steel tanks.

Drums containing the product should be kept tightly closed in a well-ventilated place.

Propylheptanol can be stored for one year at temperatures below 40 °C, if moisture is excluded.

Pumps:
Cast-steel centrifugal pumps with a simple slip-ring seal are suitable.

Flange seals:
An example of a suitable material for seals is chemical-resistant Polytetrafluoroethylene (PTFE). Other plastics should be checked for suitability before they are taken into use.

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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