

TECHNICAL DATA SHEET

Isoamyl Alcohol (3-Methyl-1-butanol), bio-based

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1 PRODUCT DESCRIPTION

Bio-based isoamyl alcohol (3-methyl-1-butanol) is obtained by distillation of fusel oil – a by-product of ethanol fermentation from sugar cane. It is chemically identical to petrochemically produced isoamyl alcohol and is suitable as a drop-in without reformulation.

Isoamyl alcohol is a colourless, clear liquid with a characteristic odour and good solvency for resins, oils and nitrocellulose. As a building block for isoamyl acetate and other esters it is a key raw material for the flavour and fragrance industry.

2 PRODUCT IDENTIFICATION

Trade name	Isoamyl alcohol, bio-based
Chemical name	3-Methylbutan-1-ol
Synonyms	Isopentyl alcohol, 3-methyl-1-butanol, isoamylol
CAS No.	123-51-3
EC No.	204-633-5
Molecular formula	C ₅ H ₁₂ O
Molecular weight	88.15 g/mol

3 TYPICAL PROPERTIES

Physical state / colour	liquid, colourless, clear
Odour	characteristic, fusel-like alcoholic
Purity (pentanols)	≥ 99.0 %
Density (20 °C)	0.81 g/cm ³
Boiling point	131 °C (1013 hPa)
Melting point	-117 °C
Flash point	43 °C (closed cup)
Auto-ignition temperature	approx. 340 °C
Explosion limits	1.2 / 9.0 vol%
Vapour pressure	approx. 3 hPa (20 °C)
Kinematic viscosity	5.3 mm ² /s (20 °C)
Water solubility	approx. 28 g/l (20 °C); miscible with ethanol, ether, acetone
log K _{ow}	1.16

Binding limits are given in the specification (PENPET_GREEN_Spec_Isoamylalkohol).

4 APPLICATIONS

- Isoamyl acetate and other flavour and fragrance esters
- Solvent for coatings, printing inks and nitrocellulose
- Pharmaceutical extraction and synthesis
- Intermediate for plasticiser and lubricant esters
- Laboratory reagent – Kovacs reagent, DNA extraction, chromatography
- Raw material for cosmetic and cleaning formulations (industrial processing)

5 REGULATORY INFORMATION

Classification (CLP)	Flam. Liq. 3 (H226), Acute Tox. 4 inhalation (H332), Skin Irrit. 2 (H315), Eye Dam. 1 (H318), STOT SE 3 (H335), Aquatic Chronic 3 (H412) · Signal word: Danger
REACH	Annex XVII: entries 3 and 40 (by virtue of the classification); not listed in Annex XIV, not on the SVHC candidate list
VOC	100 % volatile organic compound
Water hazard class (Germany)	WGK 1 (AwSV)
Storage class (Germany)	LGK 3 (TRGS 510)
Kosher	Kosher/Parve – manufacturer certificate valid until 29.07.2027

6 SUSTAINABILITY

Feedstock	Fusel oil from sugar-cane ethanol fermentation (Brazil)
Life cycle assessment	ISO 14040/14044, cradle-to-gate, EF 3.1 method; ACV Brasil, version 1.1 (March 2025); primary data 07/2023–06/2024
Review status	internally reviewed; external critical review not yet completed
Product Carbon Footprint	on request

7 PACKAGING, STORAGE AND TRANSPORT

Packaging	ISO tank container (approx. 18,000–20,000 kg), IBC (800 kg), steel drum (170 kg)
Storage	cool, dry, well ventilated, containers tightly closed; protect from heat and direct sunlight; recommended 5–30 °C
Incompatibilities	store separately from oxidising agents, strong acids and acid anhydrides
Suitable materials	stainless steel, carbon steel, HDPE
Shelf life	12 months
Transport	UN 1105 · Pentanols · Class 3 · Packing group III
Delivery	from Hamburg throughout Europe

8 AVAILABLE DOCUMENTS

- Specification (DE/EN), technical data sheet (DE/EN) and safety data sheet (DE/EN) – download at www.penpet.green
- Certificate of analysis (CoA) with every delivery
- LCA report and kosher certificate – on request

The information in this technical data sheet is based on manufacturer information and our current state of knowledge. It describes the product but does not constitute a guarantee of properties and does not release the user from carrying out their own tests. The agreed specification and the certificate of analysis of the respective delivery are binding. Information on safe handling is given in the safety data sheet.