

ISOBUTANOL

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SYNONYMS Isobutyl alcohol, IBA, isopropyl carbinol

DEFINITION

Chemical names 2-Methyl-1-propanol, 2-methylpropan-1-ol

C.A.S. number 78-83-1

Chemical formula $C_4H_{10}O$

Structural formula $(CH_3)_2CHCH_2OH$

Formula weight 74.12

Assay Not less than 99% of $C_4H_{10}O$

DESCRIPTION Clear, colourless, flammable liquid with a characteristic odour

FUNCTIONAL USES Extraction solvent, flavouring agent (see "Flavouring agents" monograph JECFA no. 251)

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4) Soluble in water; miscible with ethanol and ether

Specific gravity (Vol. 4) d_{20}^{20} : 0.802 - 0.804
 d_{25}^{25} : 0.779 - 0.801

Infrared absorption The infrared spectrum of the sample corresponds with the reference infrared spectrum below

PURITY

Water (Vol. 4) Not more than 0.2% (Karl Fischer Method)

Distillation range (Vol. 4) 106 - 109°

Colour (Vol. 4) Not more than Colour Standard No. 10

Non-volatile residue (Vol. 4) Not more than 1 mg/100 ml

Acidity Not more than 0.003% (as acetic acid)
To 60 g of the sample add a few drops of phenolphthalein TS and titrate

with 0.1 N ethanolic potassium hydroxide to a pink end-point which persists for at least 15 sec. Not more than 0.3 ml is required.

Aldehydes and ketones Not more than 0.2% (as butanal)
Proceed as directed under method *Aldehyde and Ketone Determination*, using 10 g of the sample and 36.06 as the equivalent factor (e) in the calculation.

Lead (Vol. 4) Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in Volume 4, "Instrumental Methods."

METHOD OF ASSAY Determine by *gas-liquid chromatography* (see Volume 4), using the following conditions:

Column
- length: 2.4 m
- diameter: 6 mm
- material: copper
- packing: 23% Carbowax 1500
- support: Chromosorb W (60/80 mesh)
Carrier gas: Helium
Flow rate: 150 ml/min
Detector type: FID
Temperatures
- injection port: 150°
- column: 70°
- detector: 150°

Inject 1 to 5 µl of sample, obtain chromatogram and determine content of each constituent by the method of area normalization.

Infrared spectrum Isobutanol
(Reprinted from Merck FT-IR Atlas through courtesy of Dr K.G.R. Pachler, Mr F. Matlock, and Dr H-U. Gremlich and VCH Verlagsgesellschaft, Weinheim, Germany.)

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