

TECHNICAL DATA SHEET

Isobutyl Alcohol 99% ACS Grade

ACS Grade · 99%

CAS NUMBER

78-83-1

ALLIANCE CODE

isobutyl-alcohol-99-acsg
grade

GENERATED

2026-08-31

REVISION

1.3

REVIEWED

2026-07-17 · Andre Taki

IDENTITY & COMPOSITION

PRODUCT NAME

Isobutyl Alcohol 99% ACS Grade

ALLIANCE CODE

isobutyl-alcohol-99-acsg
grade

GRADE

ACS Grade

CONCENTRATION

99%

CAS NUMBER

78-83-1 PubChem

FORMULA

C4H10O PubChem

MOLECULAR WEIGHT

74.12 PubChem

PRODUCT TYPE

solution

SPECIFICATIONS

TEST	SPECIFICATION	TYPICAL	METHOD	SOURCE
Assay (2-methyl-1-propanol)	99.0 % Min	99.0 %	Gas chromatography	ACS Reagent Chemicals
Titration acid	0.0005 meq/g Max	0.0001 meq/g	Titration with standard base	ACS Reagent Chemicals
Alkalinity	0.0005 meq/g	0.00002 meq/g	Titration with standard acid	Supplier specification

TEST	SPECIFICATION	TYPICAL	METHOD	SOURCE
Identity	IR passes test	Passes test	Infrared spectroscopy	Supplier specification
Isobutanol (G.C.)	0.05%	0.002%	Gas chromatography	Supplier specification
Peroxides (as H ₂ O ₂)	0.001%	0.0001%	Colorimetric peroxide test	Supplier specification
Residue after evaporation (non-volatile matter)	0.001 % Max	0.0002 %	Evaporation to dryness and gravimetric determination	ACS Reagent Chemicals
Insoluble matter in water (solubility in water)	passes test	Passes test	Visual examination of aqueous dilution	Supplier specification
Substances darkened by sulfuric acid	passes test	Passes test	Sulfuric acid darkening test	Supplier specification
Water (H ₂ O)	0.1 % Max	0.03 %	Karl Fischer	ACS Reagent Chemicals
Carbonyl compounds (as butyraldehyde)	0.01 % Max	0.003 %	Gas chromatography	ACS Reagent Chemicals

Specification values are guaranteed limits. Typical values are representative of production lots and are not guaranteed. Lot-specific certificates of analysis ship with every order.

AVAILABLE GRADES SAME CAS, ALTERNATE GRADES AND CONCENTRATIONS

GRADE	CONCENTRATION	TYPICAL ASSAY	SKU
THIS GRADE ACS Grade	99%	—	current

GRADE	CONCENTRATION	TYPICAL ASSAY	SKU
—	99%	—	isobutyl-alcohol-99

Typical assay shown is the rolling-window mean from the sibling product's most recent lots. Grade selection drives downstream end-use — verify the sibling grade matches your specification before substitution.

PHYSICAL & CHEMICAL PROPERTIES

One or more physical-property values are temporarily suppressed pending verification against vendor COA data. For complete properties refer to the Safety Data Sheet (SDS) or contact sales@alliancechemical.com.

PROPERTY	VALUE	SOURCE
Form	Liquid	Published reference
Color	10 Max	ACS Reagent Chemicals
Odor	Sweet, musty odor	Published reference
Density	0.801-0.802	Supplier specification
Boiling Point	107-109°C	Supplier specification
Melting Point	-162 °F (NTP, 1992)	Published reference
Flash Point	82 °F (NTP, 1992)	Published reference
Vapor Pressure	10 mmHg at 71.1 °F ; 9 mmHg at 68 °F (NTP, 1992)	Published reference
Solubility (water)	50 to 100 mg/mL at 61 °F (NTP, 1992)	Published reference
Refractive Index (nD 20)	1.397-1.399	Supplier specification

Polar solvent — purity vs. intended end-use (electronics, pharma, general industrial) is the dominant grade consideration. See application guidance for grade selection.

MATERIALS OF CONSTRUCTION

MATERIAL	RATING	CONDITIONS	SOURCE
Steel (railway tank cars, tank containers, road tankers)	Compatible	Loading and transport of isobutanol as supplied (product spec on the same page: Isobutanol >99.8 %); no temperature or concentration limit stated	grupaaazoty.com

Compatibility is drawn from published manufacturer and supplier documentation for this product; each rating is sourced. Confirm against your specific duty cycle before equipment selection.

REGULATORY & TRANSPORT

DOT / 49 CFR

UN NUMBER

UN1212 49 CFR 172.101

HAZARD CLASS

3 Adjudicated

PACKING GROUP

III Adjudicated

PROPER SHIPPING NAME

Isobutanol or isobutyl alcohol Adjudicated

GHS / OSHA HAZCOM 2012

SIGNAL WORD

Danger Adjudicated

H-CODES (HAZARD STATEMENTS)

H226, H315, H318, H335, H336 Adjudicated

P-CODES (PRECAUTIONARY STATEMENTS)

P210, P233, P240, P241, P242, P243, P261, P264, P271, P280, P302+P352, P303+P361+P353, P304+P340, P305+P351+P338, P313, P314, P321, P332+P313, P362, P370+P378, P403+P233, P403+P235, P405, P501

Adjudicated

OCCUPATIONAL EXPOSURE LIMITS

OSHA PEL (29 CFR 1910.1000)

— no canonical

ACGIH TLV

— no canonical

NIOSH REL

— no canonical

NIOSH IDLH

— no canonical

Transport descriptions reflect 49 CFR 172.101 lookup at time of publication. Sourced data: ECHA CLP Annex VI for harmonised classifications, NIOSH Pocket Guide for REL/IDLH, OSHA Z-Tables for PEL. Always verify against the latest regulatory text before shipment-critical decisions.

APPLICATIONS

Analytical reagent for laboratory analysis, meeting ACS specifications and USP / Ph. Eur. reagent requirements.

itwreagents.com

Sold for research use only, restricted to qualified laboratories and businesses. chemsavers.com

Used in organic synthesis, as a chemical intermediate, and as a solvent in coating applications.

productcatalog.eastman.com

Used in the production of esters, paints and lacquers (as solvent and flow/viscosity modifier), plasticizer additives for plastics, and melamine and carbamide resins.

grupaaazoty.com

Applications are drawn from published manufacturer and supplier documentation; each is sourced. Suitability for a specific use is the buyer's to confirm.

STORAGE & HANDLING

RECOMMENDED STORAGE

Storage: Room Temperature. itwreagents.com

INCOMPATIBILITIES

Strong oxidizers, strong acids, isocyanates, anhydrides. Hygroscopic — protect from atmospheric moisture for water-sensitive end uses.

Class-level guidance — not product-specific; the SDS controls.

For full hazard, PPE, and emergency response guidance, refer to the Safety Data Sheet (SDS) for this product. The SDS controls in all cases where guidance differs.

HANDLING PRECAUTIONS

Use chemical-resistant gloves and splash goggles. Bond and ground during transfer to prevent static accumulation. Eliminate ignition sources within vapor envelope.

Class-level guidance — not product-specific; the SDS controls.

SHELF LIFE

Consult Technical Services for product-specific shelf life

PACKAGING & LOGISTICS

SHIPPING DESCRIPTION (US DOT)

UN1212, Isobutanol or isobutyl alcohol, 3, PG III

Sourced from 49 CFR 172.101. Confirm against shipping documents and carrier requirements before tender.

NMFC CLASS 77.5	PLACARD Flammable Liquid	PACKING GROUP PG III
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REVISION HISTORY

Last reviewed 2026-07-17 by Andre Taki, DOT Hazmat Specialist.

VERSION	DATE	CHANGE	TRIGGER
1.3	2026-08-05	Canonical data updated: 1 field changed via the provenance/adjudication pipeline. unNumber · canonical change (coa.data_provenance / adjudication)	canonical_change
1.2	2026-07-22	Canonical data updated: 2 fields changed via the provenance/adjudication pipeline. - dotSubsidiaryHazardClass · canonical change (coa.data_provenance / adjudication) - dotProperShippingName · canonical change (coa.data_provenance / adjudication)	canonical_change
1.1	2026-07-17	Canonical data re-verified: 5 fields updated against independent vendor SDSs, CLP Annex VI, 49 CFR, and OSHA HazCom 2024 (GHS classification, hazard/precautionary codes, signal word, physical properties as applicable). - countryOfOrigin · canonical adjudication / reground (coa.data_provenance) - ghsClassification · canonical adjudication / reground (coa.data_provenance) - hazard_h_codes · canonical adjudication / reground (coa.data_provenance) - hazard_p_codes · canonical adjudication / reground (coa.data_provenance) - hsCode · canonical adjudication / reground (coa.data_provenance)	canonical_change
1.0	2026-05-20	Initial URL-first TDS published from canonical chemistry registry.	initial

This Technical Data Sheet is provided for technical reference. The Safety Data Sheet (SDS) controls in all cases where guidance differs. Values reflect Alliance Chemical canonical data at time of generation; subsequent revisions are recorded in the Revision History above.