Technical Data Sheet

Isobutyl Alcohol 99% ACS Grade

ACS Grade · 99%

Alliance Code	Revised	Revision
isobutyl-alcohol-99-acs-grade	2026-10-08	1.7

CAS number 78-83-1	UN number UN1212	Hazard class · packing group 3 · PG III
 Structure · PubChem	Grade ACS Grade · 99%	Signal word **Danger**

Hazards

Flammable | Corrosive | Irritant / harmful | H226 H315 H318 H335 H336

Proper shipping name

Isobutanol or isobutyl alcohol

IDENTITY & COMPOSITION

PRODUCT NAME
Isobutyl Alcohol 99% ACS Grade

ALLIANCE CODE
isobutyl-alcohol-99-acs-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	—	Gas chromatography	Interpreted
Titrable acid	0.0005 meq/g Max	—	Titration with standard base	Interpreted
Alkalinity	0.0005 meq/g	—	Titration with standard acid	Interpreted
Color (APHA)	10 Max	—	Platinum-cobalt (APHA) visual comparison	Interpreted
Identity	IR passes test	—	Infrared spectroscopy	Interpreted
Isobutanal (G.C.)	0.05%	—	Gas chromatography	Interpreted
Peroxides (as H2O2)	0.001%	—	Colorimetric peroxide test	Interpreted
Range of distillation (>96% dist.)	107-109°C	—	Distillation	Interpreted
Residue after evaporation (non-volatile matter)	0.001 % Max	—	Evaporation to dryness and gravimetric determination	Interpreted
Insoluble matter in water (solubility in water)	passes test	—	Visual examination of aqueous dilution	Interpreted
Substances darkened by sulfuric acid	passes test	—	Sulfuric acid darkening test	Interpreted
Water (H2O)	0.1 % Max	—	Karl Fischer	Interpreted
Carbonyl compounds (as butyraldehyde)	0.01 % Max	—	Gas chromatography	Interpreted

Values are reproduced from the current product reference. Source labels do not by themselves establish a supplier guarantee or a test result for your lot. Confirm applicable acceptance limits and request lot-specific documentation.

AVAILABLE GRADES SAME CAS, ALTERNATE GRADES AND CONCENTRATIONS

GRADE	CONCENTRATION	TYPICAL ASSAY	SKU
THIS GRADE ACS Grade	99%	—	current
Technical	99%	—	isobutyl-alcohol-99

Typical assay for each grade is the average of its recent lots. Confirm a grade meets your specification before substituting it.

PHYSICAL & CHEMICAL PROPERTIES

PROPERTY	VALUE	SOURCE
Appearance	Clear, colorless liquid	Adjudicated
Form	Liquid	Published reference
Odor	Alcohol-like, sweet musty odor	Adjudicated
pH	About 7 (80 g/L aqueous solution)	Adjudicated
Specific Gravity	0.80 at 20 °C (water = 1)	Adjudicated
Density	0.801-0.802	Interpreted
Boiling Point	106–108 °C (223–226 °F)	Adjudicated
Melting Point	-108 °C (-162 °F)	Adjudicated
Flash Point	28–31 °C (82–88 °F), closed cup	Adjudicated
Vapor Pressure	7–9 mmHg (9.5–12 hPa) at 20 °C	Adjudicated
Vapor Density	2.6 (air = 1)	Adjudicated
Solubility (water)	Soluble in water (70–85 g/L at 20 °C); miscible with most organic solvents	Adjudicated
Refractive Index (nD 20)	1.397-1.399	Interpreted

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	grupaazoty.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 HCS 2024

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, P310, P313, P321, P332+P313, P362, P370+P378, P403+P233, P403+P235, P405, P501

Adjudicated

OCCUPATIONAL EXPOSURE LIMITS

OSHA PEL (29 CFR 1910.1000)
100 ppm TWA OSHA 29 CFR 1910.1000

ACGIH TLV
50 ppm TWA Adjudicated

NIOSH REL
50 ppm (150 mg/m^3) TWA Adjudicated

NIOSH IDLH
1,600 ppm Adjudicated

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

HEALTH & FIRE HAZARD

ACUTE TOXICOLOGY

LD_{50} ORAL (RAT)

2,460–3,350 mg/kg (rat)

Adjudicated

LD_{50} DERMAL (RABBIT)

2,460–3,400 mg/kg

Adjudicated

LC_{50} INHALATION (RAT, 4 H)

> 18 mg/L (vapor, rat, 6 h); 24.6 mg/L (4 h)

Adjudicated

Acute toxicology values from SDS Section 11 or NIOSH RTECS.

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.

grupaazoty.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

Keep tightly closed in a cool, well-ventilated flammables area away from ignition sources and oxidizers. Store locked up. Ground and bond containers.

Adjudicated

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.

INCOMPATIBILITIES

Strong oxidizing agents and chromium(VI) oxide; alkali and alkaline-earth metals; aluminum; rubber and some plastics.

Adjudicated

SHELF LIFE

Consult Technical Services for product-specific shelf life

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.

PACKAGING & LOGISTICS

SHIPPING DESCRIPTION (US DOT)

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UN1212, Isobutanol or isobutyl alcohol, 3, PG III
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Sourced from 49 CFR 172.101. Confirm against shipping documents and carrier requirements before tender.

NMFC CLASS	PLACARD	PACKING GROUP
77.5	Flammable Liquid	PG III

REVISION HISTORY

Last reviewed 2026-10-08 by Andre Taki, Chief Commercial Officer, DOT Hazmat–certified (49 CFR 172.704).

VERSION	DATE	CHANGE	TRIGGER
1.7	2026-10-08	Canonical data updated: 24 fields changed via the provenance/adjudication pipeline. • synonyms · canonical change (coa.data_provenance / adjudication) • restrictions_on_use · canonical change (coa.data_provenance / adjudication) • odor · canonical change (coa.data_provenance / adjudication) • pH · canonical change (coa.data_provenance / adjudication) • flashPoint · canonical change (coa.data_provenance / adjudication) • boilingPoint · canonical change (coa.data_provenance / adjudication) • meltingPoint · canonical change (coa.data_provenance / adjudication) • vaporPressure · canonical change (coa.data_provenance / adjudication) • vaporDensity · canonical change (coa.data_provenance / adjudication) • specificGravity · canonical change (coa.data_provenance / adjudication) • solubility · canonical change (coa.data_provenance / adjudication) • autoIgnitionTemperature · canonical change (coa.data_provenance / adjudication) • explosiveLimits · canonical change (coa.data_provenance / adjudication) • oel_acgih_tlv · canonical change (coa.data_provenance / adjudication) • oel_niosh_rel · canonical change (coa.data_provenance / adjudication) • oel_idlh · canonical change (coa.data_provenance / adjudication) • incompatible_materials · canonical change (coa.data_provenance / adjudication) • conditions_to_avoid · canonical change (coa.data_provenance / adjudication) • hazardous_decomposition_products · canonical change (coa.data_provenance / adjudication) • storage_precautions · canonical change (coa.data_provenance / adjudication) • rcra_waste_codes · canonical change (coa.data_provenance / adjudication) • cercla_rq · canonical change (coa.data_provenance / adjudication) • dot_transport_note · canonical change (coa.data_provenance / adjudication) • recommended_use · canonical change (coa.data_provenance / adjudication)	canonical_change
1.6	2026-10-07	Canonical data updated: 3 fields changed via the provenance/adjudication pipeline. • ghsClassification · canonical change (coa.data_provenance / adjudication) • hazard_h_codes · canonical change (coa.data_provenance / adjudication) • hazard_p_codes · canonical change (coa.data_provenance / adjudication)	canonical_change
1.5	2026-10-05	Canonical data updated: 3 fields changed via the provenance/adjudication pipeline. • oel_niosh_rel · canonical change (coa.data_provenance / adjudication) • oel_idlh · canonical change (coa.data_provenance / adjudication) • oel_osha_pel · canonical change (coa.data_provenance / adjudication)	canonical_change

VERSION	DATE	CHANGE	TRIGGER
1.4	2026-09-30	Canonical data updated: 4 fields changed via the provenance/adjudication pipeline. • boilingPoint · canonical change (coa.data_provenance / adjudication) • meltingPoint · canonical change (coa.data_provenance / adjudication) • flashPoint · canonical change (coa.data_provenance / adjudication) • appearance · canonical change (coa.data_provenance / adjudication)	canonical_change
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.