

TECHNICAL DATA SHEET

Isopropyl Acetate 99.98% ACS Grade

ACS Grade · 99.98%

CAS NUMBER

108-21-4

ALLIANCE CODE

isopropyl-acetate-99-98-
acs-grade

GENERATED

2026-08-31

REVISION

1.3

REVIEWED

2026-07-17 · Andre Taki

IDENTITY & COMPOSITION

PRODUCT NAME

Isopropyl Acetate 99.98% ACS Grade

ALLIANCE CODE

isopropyl-acetate-99-98-acs-grade

GRADE

ACS Grade

CONCENTRATION

99.98%

CAS NUMBER

108-21-4 [PubChem](#)

FORMULA

C₅H₁₀O₂ [PubChem](#)

MOLECULAR WEIGHT

102.13 [PubChem](#)

PRODUCT TYPE

solution

IUPAC NAME

propan-2-yl acetate [PubChem](#)

INCHI-KEY

JMMWKBVZLWUJPJ-UHFFFA0YSA-N [PubChem](#)

SMILES

CC(C)OC(=O)C [PubChem](#)

PHARMACOPOEIA COMPLIANCE: [ACS](#)

SPECIFICATIONS

TEST	SPECIFICATION	TYPICAL	METHOD	SOURCE
Assay (isopropyl acetate)	99.5 % min.	100.0 %	GC	Supplier specification

TEST	SPECIFICATION	TYPICAL	METHOD	SOURCE
Acidity (as acetic acid)	0.005 wt % max.	0.0008 wt %	—	Supplier specification
Copper (Cu)	0.02 ppm max.	0.002 ppm	—	Supplier specification
Identification	Conforms	Passes test	FTIR	Supplier specification
Iron (Fe)	0.1 ppm max.	0.02 ppm	—	Supplier specification
Nickel (Ni)	0.02 ppm max.	0.002 ppm	—	Supplier specification
Lead (Pb)	0.1 ppm max.	0.005 ppm	—	Supplier specification
Non-volatile matter	0.002 % max.	0.0003 %	—	Supplier specification
Water	0.05 % max.	0.015 %	Karl Fischer	Supplier specification
Isopropanol (free alcohol)	0.1 % max.	0.01 %	GC-FID (ASTM D3545)	Interpreted
Substances darkened by sulfuric acid	Passes test	Passes test	ACS reagent method	Interpreted

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	99.98%	—	current
Technical	99.98%	—	isopropyl-acetate-99-98

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

PROPERTY	VALUE	SOURCE
Appearance	Clear colorless	Supplier specification
Form	Liquid	Published reference
Color	5 max.	Supplier specification
Odor	Aromatic	Published reference
Specific Gravity (20 °C)	0.872 – 0.874	JECFA monograph
Density	0.874 at 68 °F (USCG, 1999) – Less dense than water; will float	Published reference
Boiling Point	87 – 90 °C	Interpreted
Melting Point	–100.1 °F (NTP, 1992)	Published reference
Flash Point	36 °F (NTP, 1992)	Published reference
Vapor Pressure	1 mmHg at –36.9 °F ; 100 mmHg at 96.3 °F; 760 mmHg at 192.2 °F (NTP, 1992)	Published reference
Solubility (water)	1 to 10 mg/mL at 68 °F (NTP, 1992)	Published reference
Refractive Index (nD 20)	1.376 – 1.378	Supplier specification

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

MATERIAL	RATING	MAX T (°C)	NOTES	SOURCE
Buna-N (NBR) Elastomer	Fair	60	Acceptable for alcohols; poor for ketones.	Parker O-ring Chemical Compatibility
EPDM Elastomer	Fair	—	Good for alcohols, poor for esters	Cole-Parmer Chemical Compatibility
Viton (FKM) Elastomer	Fair	80	Swells in acetone and esters; avoid for those.	Parker O-ring Chemical Compatibility
FFKM (Kalrez) Fluoropolymer	Excellent	200	Premium ester / ketone sealing	Cole-Parmer Chemical Compatibility
PTFE Fluoropolymer	Excellent	200	Universal solvent compatibility.	Cole-Parmer Chemical Compatibility
Borosilicate Glass Glass Ceramic	Excellent	100	Universally inert.	Cole-Parmer Chemical Compatibility
Glass (borosilicate) Glass Ceramic	Excellent	100	Inert	Cole-Parmer Chemical Compatibility
316L Stainless Steel Metal	Excellent	80	Inert; preferred for high-purity solvent service.	Cole-Parmer Chemical Compatibility
Aluminium Metal	Good	40	Acceptable; avoid prolonged wet contact	Cole-Parmer Chemical Compatibility
Carbon Steel Metal	Fair	50	Trace moisture causes rust; flash-rust prevention required.	Cole-Parmer Chemical Compatibility
HDPE Thermoplastic	Fair	40	Swells with many polar solvents; verify per solvent.	Cole-Parmer Chemical Compatibility

MATERIAL	RATING	MAX T (°C)	NOTES	SOURCE
PP Thermoplastic	Good	50	Acceptable but watch swelling with esters	Cole-Parmer Chemical Compatibility
PVC Thermoplastic	Fair	25	Esters soften PVC; avoid for esters	Cole-Parmer Chemical Compatibility

Ratings reflect the service envelope (concentration × temperature) shown. Always confirm against your specific duty cycle and contact-time before equipment selection. The most cautious rating across overlapping references is shown.

REGULATORY & TRANSPORT

DOT / 49 CFR

UN NUMBER

UN1220 [49 CFR 172.101](#)

PACKING GROUP

II [Adjudicated](#)

HAZARD CLASS

3 [Adjudicated](#)

PROPER SHIPPING NAME

Isopropyl acetate [Adjudicated](#)

GHS / OSHA HAZCOM 2012

SIGNAL WORD

Danger [Adjudicated](#)

H-CODES (HAZARD STATEMENTS)

H225, H319, H336 [Adjudicated](#)

P-CODES (PRECAUTIONARY STATEMENTS)

P210, P233, P240, P241, P242, P243, P261, P264, P271, P280, P303+P361+P353, P304+P340, P305+P351+P338, P314, P337+P313, 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](#)

REGIONAL CLASSIFICATIONS

EC NUMBER (EU EINECS)

203-561-1 [Web SDS consensus](#)

REACH SVHC

Not listed [Web SDS consensus](#)

CALIFORNIA PROP 65

Not listed [Web SDS consensus](#)

WGK WATER HAZARD (DE)

1 [Web SDS consensus](#)

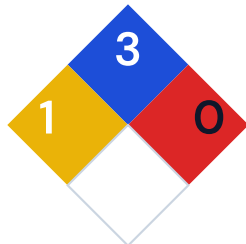
TDG CLASSIFICATION (CANADA)

un1220, class 3, pg ii [Web SDS consensus](#)

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.

HEALTH & FIRE HAZARD

NFPA 704



- Health: 1 [Web SDS consensus](#)
- Fire: 3 [Web SDS consensus](#)
- Reactivity: 0 [Web SDS consensus](#)
- Specific: —

HMIS III

Health	1	Web SDS consensus
Flammability	3	Web SDS consensus
Physical Hazard	0	Web SDS consensus
PPE	B	Web SDS consensus

ACUTE TOXICOLOGY

LD₅₀ ORAL (RAT)
6750 mg/kg [Web SDS consensus](#)

LC₅₀ INHALATION (RAT, 4 H)
32500 mg/m³ [Web SDS consensus](#)

NFPA 704 ratings 0 (no hazard) – 4 (severe hazard) per NFPA 704 standard. HMIS III ratings 0 – 4 per the American Coatings Association. Acute toxicology values from SDS Section 11 or NIOSH RTECS.

CATALOG EQUIVALENTS CROSS-REFERENCE VS MAJOR CHEMICAL SUPPLIERS

SIGMA-ALDRICH

SKU	GRADE	CONC.	MATCH	NOTES
109584	ACS reagent	≥99.5%	Exact	Same ACS reagent grade.

Cross-references are informational. Confirm against the manufacturer's current specification before substitution. Competitor trademarks are property of their respective owners.

APPLICATIONS

General-purpose fast-evaporating solvent, miscible with most common organic solvents, with properties between ethyl and butyl acetate

[stobec.com](#)

Active solvent for synthetic resins including cellulose acetate butyrate, nitrocellulose, vinyl copolymers, polyesters, polyamides, acrylics and alkyds

[stobec.com](#)

Solvent in coatings: automotive OEM and refinish, can and coil, general industrial, industrial maintenance and marine, industrial wood, transportation

[stobec.com](#)

Fragrance carrier in cosmetics and personal care, and solvent in flexographic and gravure printing inks

stobec.com

Solvent for cellulose, plastics, oils and fats; component of some printing inks and perfumes

corecheminc.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

Cool, well-ventilated flammable-liquid storage area. Tightly sealed original containers. Segregate from oxidizers and acids. Bond and ground bulk storage.

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

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)

UN1220, Isopropyl acetate, 3, PG II

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

NMFC CLASS
70

PLACARD
Flammable Liquid

PACKING GROUP
PG II

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: 3 fields changed via the provenance/adjudication pipeline. • hazardClass · canonical change (coa.data_provenance / adjudication) • packingGroup · canonical change (coa.data_provenance / adjudication) • unNumber · canonical change (coa.data_provenance / adjudication)	canonical_change
1.2	2026-07-22	Canonical data updated: 1 field changed via the provenance/adjudication pipeline. • dotSubsidiaryHazardClass · canonical change (coa.data_provenance / adjudication)	canonical_change

VERSION	DATE	CHANGE	TRIGGER
1.1	2026-07-17	Canonical data re-verified: 25 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). - acs_compliance · canonical adjudication / reground (coa.data_provenance) - countryOfOrigin · canonical adjudication / reground (coa.data_provenance) - ec_number · 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) - hmis_flammability · canonical adjudication / reground (coa.data_provenance) - hmis_health · canonical adjudication / reground (coa.data_provenance) - hmis_physical · canonical adjudication / reground (coa.data_provenance) - hmis_ppe · canonical adjudication / reground (coa.data_provenance) - hsCode · canonical adjudication / reground (coa.data_provenance) - inchi · canonical adjudication / reground (coa.data_provenance) - inchi_key · canonical adjudication / reground (coa.data_provenance) - iupac_name · canonical adjudication / reground (coa.data_provenance) - lc50_inhalation_rat_4h · canonical adjudication / reground (coa.data_provenance) - ld50_oral_rat · canonical adjudication / reground (coa.data_provenance) - nfpa_fire · canonical adjudication / reground (coa.data_provenance) - nfpa_health · canonical adjudication / reground (coa.data_provenance) - nfpa_reactivity · canonical adjudication / reground (coa.data_provenance) - prop_65_listed · canonical adjudication / reground (coa.data_provenance) - pubchem_cid · canonical adjudication / reground (coa.data_provenance) - reach_svhc_listed · canonical adjudication / reground (coa.data_provenance) - smiles · canonical adjudication / reground (coa.data_provenance) - tdg_classification · canonical adjudication / reground (coa.data_provenance) - wgk_water_hazard · canonical adjudication / reground (coa.data_provenance)	canonical_change

VERSION	DATE	CHANGE	TRIGGER
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.