

• SAFETY DATA SHEET

Version 6.8
Revision Date 12/26/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : *tert*-Butan(ol-d)

Product Number : 175765
Brand : Aldrich
CAS-No. : 3972-25-6

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 2

Acute toxicity (Inhalation) : Category 4


Eye irritation : Category 2A

Specific target organ toxicity - single exposure : Category 3 (Respiratory system, Central nervous system)

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H332 Harmful if inhaled.
H335 May cause respiratory irritation.
H336 May cause drowsiness or dizziness.

Precautionary statements : **Prevention:**
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P261 Avoid breathing mist or vapours.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P337 + P313 If eye irritation persists: Get medical advice/ attention.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P403 + P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 3972-25-6

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
tert-Butyl alcohol-d	3972-25-6*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Immediately call in physician.
If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact : After eye contact: rinse out with plenty of water.
Call in ophthalmologist.
Remove contact lenses.

If swallowed : After swallowing: immediately make victim drink water (two glasses at most).
Consult a physician.

Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Carbon dioxide (CO ₂) Foam Dry powder
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Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
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Specific hazards during fire fighting	: Combustible.
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Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

Hazardous combustion products	: Carbon oxides
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Specific extinguishing methods	: No data available
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Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
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Special protective equipment for fire-fighters : In the event of fire, wear self-contained breathing apparatus.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapours, aerosols.
Avoid substance contact.
Ensure adequate ventilation.
Keep away from heat and sources of ignition.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.
Risk of explosion.

Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.
Keep away from heat and sources of ignition.

Storage class : 3, Flammable liquids

Recommended storage temperature : Recommended storage temperature see product label.

Packaging material : Suitable material: Mild Steel Drum

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
tert-Butyl alcohol-d	3972-25-6	TWA	100 ppm	ACGIH
		TWA	100 ppm 300 mg/m ³	NIOSH REL
		ST	150 ppm 450 mg/m ³	NIOSH REL
		TWA	100 ppm 300 mg/m ³	OSHA Z-1

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.4 mm
Protective index : Full contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Material : Chloroprene
Break through time : 240 min
Glove thickness : 0.65 mm
Protective index : Splash contact
Manufacturer : KCL 720 Camapren®

Remarks	: This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Eye protection	: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	: Flame retardant antistatic protective clothing.
Hygiene measures	: Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid
Color	: No data available
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: 73 - 79 °F / 23 - 26 °C Method: lit.
Boiling point/boiling range	: 181 °F / 83 °C Method: lit.
Flash point	: 52 °F / 11 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit /	: 8.0 %(V)

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Upper flammability limit	
Lower explosion limit / Lower flammability limit	: 2.3 %(V)
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 0.786 g/cm ³ (77 °F / 25 °C)
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 75.13 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapours may form explosive mixture with air.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: Alkali metals Alkaline earth metals Strong acids Aluminium

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Strong oxidizing agents

Conditions to avoid : Warming.

Incompatible materials : No data available

Hazardous decomposition : In the event of fire: see section 5 products

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 3,046 mg/kg
(US-EPA)

Remarks: The value is given in analogy to the following substances: tert-Butanol
Acute toxicity estimate Inhalation - 4 h - 11.1 mg/l - vapour

(Expert judgement)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: tert-Butanol

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

(US-EPA)

Remarks: The value is given in analogy to the following substances: tert-Butanol

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

(Draize Test)

Remarks: The value is given in analogy to the following substances: tert-Butanol

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(US-EPA)

Remarks: The value is given in analogy to the following substances: tert-Butanol

Respiratory or skin sensitization

Maximisation Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: tert-Butanol

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol

Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

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Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol
Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol
Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 479

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: tert-Butanol

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: tert-Butanol

Inhalation - May cause drowsiness or dizziness. - Nervous system

Remarks: The value is given in analogy to the following substances: tert-Butanol

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

drying, cracking of the skin, Skin irritation

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

tert-Butyl alcohol-d:

Toxicity to fish	: LC50 (Pimephales promelas (fathead minnow)): > 961 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: tert-Butanol
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 933 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: Directive 67/548/EEC, Annex V, C.2. GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: tert-Butanol
Toxicity to algae/aquatic plants	: ErC50 (Pseudokirchneriella subcapitata (green algae)): > 976 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: tert-Butanol
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: EC50 (Daphnia magna (Water flea)): > 100 mg/l End point: Immobilization Exposure time: 21 d Test Type: semi-static test

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Analytical monitoring: yes
Method: OECD Test Guideline 211
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: tert-Butanol

NOEC (Daphnia magna (Water flea)): 100 mg/l
End point: Immobilization
Exposure time: 21 d
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 211
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: tert-Butanol

Toxicity to microorganisms

: EC50 (Pseudomonas putida): > 10,000 mg/l
Exposure time: 16 h
Test Type: static test
Method: DIN 38 412 Part 8
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: tert-Butanol

EC10 (Pseudomonas putida): 6,900 mg/l
Exposure time: 16 h
Test Type: static test
Method: DIN 38 412 Part 8
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: tert-Butanol

Persistence and degradability

Components:

tert-Butyl alcohol-d:

Biodegradability : aerobic
Concentration: 30.9 mg/l
Result: Inherently biodegradable.
Biodegradation: 66 %
Exposure time: 56 d
GLP: yes
Remarks: (ECHA)

The value is given in analogy to the following substances:

The value is given in analogy to the following substances: tert-Butanol

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 1120
Proper shipping name : Butanols
Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
Packing instruction (cargo aircraft) : 364
Packing instruction (passenger aircraft) : 353

IMDG-Code

UN number : UN 1120
Proper shipping name : BUTANOLS

Class : 3
Packing group : II
Labels : 3
EmS Code : F-E, S-D
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 1120
Proper shipping name : Butanols

Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
ERG Code : 129
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION**CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

tert-Butyl alcohol-d	3972-25-6	>= 90 - <= 100 %
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US State Regulations**Massachusetts Right To Know**

tert-Butyl alcohol-d	3972-25-6
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Pennsylvania Right To Know

tert-Butyl alcohol-d	3972-25-6
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Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

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Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	: USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	: USA. NIOSH Recommended Exposure Limits
OSHA Z-1	: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	: 8-hour, time-weighted average
NIOSH REL / TWA	: Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / ST	: STEL - 15-minute TWA exposure that should not be exceeded at any time during a workday
OSHA Z-1 / TWA	: 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development;

OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Details in analogy to the undeuterated compound.

Revision Date : 12/26/2025

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