

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision
Supersedes Version

3.02
3.01***

Revision Date
Issuing date

10-Feb-2021
10-Feb-2021

SECTION 1: Identification of the substance / mixture and of the company / undertaking

1.1. Product identifier

Identification of the
substance/preparation

2-Methylbutanal

CAS-No
EC No.

96-17-3
202-485-6

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

Use of the Substance /
Preparation

Intermediate.

Uses advised against

None

1.3. Details of the supplier of the safety data sheet

Company/Undertaking
Identification

OQ Chemicals GmbH
Rheinpromenade 4A
D-40789 Monheim
Germany

Product Information

Product Stewardship
FAX: +49 (0)208 693 2053
email: sc.psq@oq.com

1.4. Emergency telephone number

Emergency telephone number

+44 (0) 1235 239 670 (UK) available 24/7
NCEC +1 202 464 2554 available 24/7

Local emergency telephone
number

+61 2 8014 4558 (Australia)
18000 74234 (Australia toll-free number)
+64 9 929 1483 (New Zealand)
0800 446 881 (New Zealand toll-free number)
+65 3158 1195 (Sri Lanka)
007 803 011 0293 (Indonesia toll-free number)
+60 3 6207 4347 (Malaysia)
001 800 120 666 751 (Thailand toll-free number)
+65 3158 1200 (Bangladesh)
+63 2 8231 2149 (Philippines)
+84 28 4458 2388 (Vietnam)
+65 3165 2217 (Singapore)
available 24/7

SECTION 2: Hazards identification

Europe

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

2.1. Classification of the substance or mixture

This substance is classified based on Directive 1272/2008/EC and its amendments (CLP Regulation)

Flammable liquid Category 2, H225
Serious eye damage/eye irritation Category 2, H319
Skin sensitization Category 1, H317
Target Organ Systemic Toxicant - Single exposure Category 3, H335
Environmental hazard Aquatic Chronic 2; H411

Additional information

For full text of Hazard- and EU Hazard-statements see SECTION 16.

2.2. Label elements

Labelling according to Regulation 1272/2008/EC and its amendments (CLP Regulation).

Hazard pictograms



Signal word

Danger

Hazard statements

H225: Highly flammable liquid and vapour.
H319: Causes serious eye irritation.
H317: May cause an allergic skin reaction.
H335: May cause respiratory irritation.
H411: Toxic to aquatic life with long lasting effects.

Precautionary statements

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233: Keep container tightly closed.
P261: Avoid breathing gas/mist/vapours.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P403 + P235: Store in a well ventilated place. Keep cool.
P501: Dispose of contents/container in accordance with local regulation.

2.3. Other hazards

Vapours may form explosive mixture with air

Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

PBT and vPvB assessment Not required

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

USA

2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

Serious eye damage/eye irritation Category 2A, H319
Skin sensitization Category 1, H317
Target Organ Systemic Toxicant - Single exposure Category 3, H335
Flammable liquid Category 2, H225
Environmental hazard Aquatic Acute 2; H401; Aquatic Chronic 2; H411

OSHA Specified Hazards Not applicable.

2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).

Hazard symbol(s)



Signal word

Danger

Hazard statements

H225: Highly flammable liquid and vapor.
H319: Causes serious eye irritation.
H317: May cause an allergic skin reaction.
H335: May cause respiratory irritation.
H411: Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233: Keep container tightly closed.
P241: Use explosion-proof electrical/ ventilating/ lighting equipment.
P242: Use non-sparking tools.
P243: Take precautionary measures against static discharge.
P261: Avoid breathing gas/mist/vapours.
P264: Wash hands thoroughly after handling.
P271: Use only outdoors or in a well ventilated area.
P272: Contaminated work clothing must not be allowed out of the workplace.
P273: Avoid release to the environment.
P280: Wear protective gloves/eye protection/face protection.

Response

P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P333 + P313: If skin irritation or rash occurs: Get medical advice/attention.
P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313: If eye irritation persists: Get medical advice/ attention.
P363: Wash contaminated clothing before reuse.
P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P312: Call a POISON CENTRE/doctor if you feel unwell.
P391: Collect spillage.

Storage P403 + P235: Store in a well ventilated place. Keep cool.
P405: Store locked up.

Disposal P501: Dispose of contents/container in accordance with local regulation.

2.3. Other hazards

None known

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	REACH-No	1272/2008/EC	Concentration (%)
2-Methylbutyraldehyde	96-17-3	01-2119615422-50	Flam. Liq. 2; H225 Eye Irrit. 2; H319 Skin Sens. 1; H317 STOT SE 3; H335 Aquatic Chronic 2; H411	> 98,0

SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

Eyes

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Obtain medical attention.

Skin

Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

Ingestion

Do not induce vomiting without medical advice. Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

Main symptoms

shortness of breath, headache, nausea, vomiting.

Special hazard

Lung oedema, Lung irritation.



2-Methylbutanal
10790

Version / Revision 3.02

4.3. Indication of any immediate medical attention and special treatment needed

General advice

Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. In case of lung irritation, first treatment with cortisone spray.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

alcohol-resistant foam, dry chemical, carbon dioxide (CO₂), water spray

Unsuitable Extinguishing Media

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

Under conditions giving incomplete combustion, hazardous gases produced may consist of:

carbon monoxide (CO)

carbon dioxide (CO₂)

Combustion gases of organic materials must in principle be graded as inhalation poisons

Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback

Vapours may form explosive mixture with air

5.3. Advice for firefighters

Special protective equipment for firefighters

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

Precautions for firefighting

Cool containers / tanks with water spray. Dike and collect water used to fight fire. Keep people away from and upwind of fire. Water run-off can cause environmental damage.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel: For personal protective equipment see section 8. Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition.

For emergency responders: Personal protection see section 8.

6.2. Environmental precautions

Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant). Water runoff can cause environmental damage.

6.3. Methods and material for containment and cleaning up

Methods for containment

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

Methods for cleaning up

Soak up with inert absorbent material. DO NOT use combustible materials such as sawdust. If liquid has been spilled in large quantities clean up promptly by scoop or vacuum. Keep in suitable, closed containers for disposal. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

6.4. Reference to other sections

For personal protective equipment see section 8.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms. Refill and handle product only in closed system. Do not use compressed air for filling, discharging or handling.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Advice on the protection of the environment

See Section 8: Environmental exposure controls.

Incompatible products

acids and bases
amines
oxidizing agents

7.2. Conditions for safe storage, including any incompatibilities

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material. Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback. Vapours may form explosive mixture with air.

Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Handle under nitrogen, protect from moisture. Store at temperatures not exceeding 38 °C/ 100 °F.

Suitable material

stainless steel

Unsuitable material

mild steel

Temperature class

T4

7.3. Specific end use(s)



2-Methylbutanal
10790

Version / Revision 3.02

Transported isolated intermediate (1907/2006)

SECTION 8: Exposure controls / personal protection

8.1. Control parameters

Exposure limits European Union

No exposure limits established

Exposure limits Germany

No exposure limits established.

Exposure limits United States of America

No exposure limits established.

8.2. Exposure controls

Appropriate Engineering controls

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

Personal protective equipment

General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

Eye protection

Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.

Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

Suitable material	butyl-rubber
Evaluation	according to EN 374: level 3
Glove thickness	approx 0.3 mm
Break through time	approx 60 min

Suitable material	polyvinylchloride
Evaluation	Information derived from practical experience
Glove thickness	approx 0.8 mm

Skin and body protection

Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

Respiratory protection

Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (dust). Equipment should conform to NIOSH, EN or other applicable national standards.

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. Observe the exposure limits, clean exhaust air if needed. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	liquid
Colour	colourless
Odour	strong
Odour threshold	1 ppb
pH	3,2 (13 g/l in water @ 20 °C (68 °F)) OECD 105
Melting point/range	< -90 °C (Pour point) @ 1013 hPa
Boiling point/range	92 °C @ 1013 hPa
Flash point	-5 °C @ 1013 hPa
Method	EU A.9
Evaporation rate	No data available
Flammability (solid, gas)	Does not apply, the substance is a liquid
Lower explosion limit	No data available
Upper explosion limit	No data available

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
76	7,6	0,075	20	68	DIN EN 13016-2
259	25,9	0,256	50	122	DIN EN 13016-2

Vapour density No data available

Relative density

Values	@ °C	@ °F	Method
0,803	20	68	DIN 51757

Solubility 13 g/l @ 20 °C, in water, OECD 105

log Pow 1,23 (calculated), KOW WIN

Autoignition temperature 190 °C @ 1017 hPa

Method DIN 51794

Decomposition temperature No data available

Viscosity 0,66 mm²/s @ 20°C

Method OECD 114, kinematic

Oxidizing properties Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties

Explosive properties Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties

9.2. Other information

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

Molecular weight 86,13
Molecular formula C₅ H₁₀ O
log K_{oc} 0,45 - 1,37 calculated
Refractive index 1,39 @ 20 °C
Surface tension 48,8 mN/m (1 g/l @ 20°C (68°F)), OECD 115

SECTION 10: Stability and Reactivity

10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous reactions occur in the presence of acids, base or oxidizing agents. This reaction is exothermic and may create heat. When finely distributed, self-ignition is possible. May form explosive peroxides.***

10.4. Conditions to avoid

Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

10.5. Incompatible materials

bases, amines, acids, oxidizing agents.

10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure Ingestion, Inhalation, Eye contact, Skin contact

Acute toxicity				
2-Methylbutyraldehyde (96-17-3)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	6884 mg/kg	rat male	OECD 401
Dermal	LD50	5400 mg/kg	rabbit male	OECD 402
Inhalative	LC50	50,5 mg/l (4h)	rat	OECD 403

2-Methylbutyraldehyde, CAS: 96-17-3

Assessment

Based on available data, the classification criteria are not met for:

Acute oral toxicity

Acute dermal toxicity

Acute inhalation toxicity

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

Irritation and corrosion				
2-Methylbutyraldehyde (96-17-3)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	Moderate skin irritation	OECD 404	read across 4h
Eyes	rabbit	irritating		read across

2-Methylbutyraldehyde, CAS: 96-17-3

Assessment

The available data lead to the classification given in section 2
For respiratory irritation, no data are available

Sensitization				
2-Methylbutyraldehyde (96-17-3)				
Target Organ Effects	Species	Evaluation	Method	
Skin	mouse	sensitizing	OECD 429	

2-Methylbutyraldehyde, CAS: 96-17-3

Assessment

Based on available data, the classification criteria are not met for:
For respiratory sensitization, no data are available

Subacute, subchronic and prolonged toxicity				
2-Methylbutyraldehyde (96-17-3)				
Type	Dose	Species	Method	
Chronic toxicity	NOAEC: 500 ppm (24 month)	rat mouse	OECD 453 Inhalation	read across

2-Methylbutyraldehyde, CAS: 96-17-3

Assessment

Based on available data, the classification criteria are not met for:
STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity					
2-Methylbutyraldehyde (96-17-3)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative (without metabolic activation)	OECD 471 (Ames)	In vitro study read across
Mutagenicity		V79 cells, Chinese hamster	positive (without metabolic activation)	OECD 476 (Mammalian Gene Mutation) HPRT	In vitro study read across
Mutagenicity		rat, hepatocytes	positive	OECD 482 UDS test	In vitro study read across
Mutagenicity		human hepatocytes	negative	OECD 482 UDS test	In vitro study read across
Mutagenicity		mouse	negative	OECD 474 Micronucleus	in vivo read across
Reproductive toxicity	No data available				
Carcinogenicity	NOAEC: 2000 ppm	rat mouse	negative	OECD 453 Inhalation	in vivo read across

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

2-Methylbutyraldehyde, CAS: 96-17-3

CMR Classification

The available data on CMR properties do not indicate a classification into categories 1A or 1B

Evaluation

Did not show carcinogenic effects in animal experiments

2-Methylbutyraldehyde, CAS: 96-17-3

Main symptoms

shortness of breath, headache, nausea, vomiting.

Target Organ Systemic Toxicant - Single exposure

STOT SE

respiratory system

The available data lead to the classification given in section 2

Target Organ Systemic Toxicant - Repeated exposure

Based on available data, the classification criteria are not met for:

STOT RE

Aspiration toxicity

Due to the viscosity, this product does not present an aspiration hazard

Other adverse effects

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin.

Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:

<http://echa.europa.eu/information-on-chemicals/registered-substances>.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity			
2-Methylbutyraldehyde (96-17-3)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	48h	EC50: 7,2 mg/l	OECD 202
Pseudokirchneriella subcapitata	72h	EC50: 123 mg/l (Growth rate)	OECD 201
Pimephales promelas (fathead minnow)	96h	LC50: 9.97 mg/l	

Long term toxicity				
2-Methylbutyraldehyde (96-17-3)				
Type	Species	Dose	Method	
Aquatic toxicity	Pseudokirchneriella subcapitata	NOEC: 1,43 mg/l (3d) Growth inhibition	OECD 201	

12.2. Persistence and degradability

2-Methylbutyraldehyde, CAS: 96-17-3

Biodegradation

54,2 % (28 d), Sewage, aerobic, OECD 301 D.

Abiotic Degradation

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

2-Methylbutyraldehyde (96-17-3)		
Type	Result	Method
Hydrolysis	not expected	
Photolysis	Half-life (DT50): 14,32 h	SRC AOP v1.92

12.3. Bioaccumulative potential

2-Methylbutyraldehyde (96-17-3)		
Type	Result	Method
log Pow	1,23	calculated, KOW WIN
BCF	No data available	

12.4. Mobility in soil

2-Methylbutyraldehyde (96-17-3)		
Type	Result	Method
Surface tension	48,8 mN/m (1 g/l @ 20°C (68°F))	OECD 115
Distribution to environmental compartments	Air: 6,52% Soil: 41,2% Water: 52,2%,	Calculation according Mackay, Level III
Adsorption/Desorption	log Koc: 0,45 - 1,37 calculated	

12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Note

Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product Information

Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

Hazardous waste according to European Waste Catalogue (EWC)

Uncleaned empty packaging

Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

SECTION 14: Transport information

ICAO-TI / IATA-DGR

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

14.1. UN number	UN 3371
14.2. UN proper shipping name	2-Methylbutanal
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	no data available

IMDG

14.1. UN number	UN 3371
14.2. UN proper shipping name	2-Methylbutanal
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
EmS	F-E, S-D
14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code	
Product name	Valeraldehyde
Ship type	3
Pollution category	Y

ADR/RID

14.1. UN number	UN 3371
14.2. UN proper shipping name	2-Methylbutanal
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
ADR Tunnel restriction code	(D/E)
Classification Code	F1
Hazard Number	33

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

DI 2012/18/EU (Seveso III)

Category	Annex I, part 1: P5a - c; depending on conditions E2
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DI 1999/13/EC (VOC Guideline)

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

Component	Status
2-Methylbutyraldehyde CAS: 96-17-3	regulated

International Inventories

2-Methylbutyraldehyde, CAS: 96-17-3

AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2024856 (EU)
ENCS (2)-494 (JP)
ISHL (2)-494 (JP)
KECI KE-23535 (KR)
INSQ (MX)
PICCS (PH)
TSCA (US)
NZIoC-NZ May be used as single component chemical
TCSI (TW)

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3

H225: Highly flammable liquid and vapour.
H319: Causes serious eye irritation.
H317: May cause an allergic skin reaction.
H335: May cause respiratory irritation.
H411: Toxic to aquatic life with long lasting effects.

Abbreviations

A table of terms and abbreviations can be found under the following link:
http://echa.europa.eu/documents/10162/13632/information_requirements_r20_en.pdf

Training advice

For effective first-aid, special training / education is needed.

Sources of key data used to compile the datasheet

Information contained in this safety data sheet is based on OQ owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/EC indicates, that no data meeting these requirements is available.

Further information for the safety data sheet

Changes against the previous version are marked by ***. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the OQ homepage (www.chemicals.oq.com).

The annex is not required because the substance is registered as an intermediate under REACH

Disclaimer

For industrial use only. The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. OQ makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

SAFETY DATA SHEET



2-Methylbutanal
10790

Version / Revision 3.02

End of Safety Data Sheet