



Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH)

Revision date: 27.12.2017

Version: 7.0

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

1.1 Product identifier

Trade name/designation:	2,2,4-Trimethylpentane, dehydrated (max. 0.01% H ₂ O) GPR RECTAPUR® for synthesis
Product No.:	28780
CAS No.:	540-84-1
INDEX No.:	601-009-00-8
REACH No.:	Not yet communicated down the supply chain.
Other means of identification:	no data available

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

Relevant identified uses:	General chemical reagent
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1.3 Details of the supplier of the safety data sheet

United Kingdom

VWR International Ltd.

Street	Hunter Boulevard, Magna Park
Postal code/city	Lutterworth, LE17 4XN
Telephone	0800 22 33 44
Telefax	01455 55 85 86
E-mail (competent person)	SDS@vwr.com

Emergency telephone

Telephone	+44 (0) 1270 502894 (CareChem24)
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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

2.1.1 Classification according to Regulation (EC) No. 1272/2008 [CLP]

Hazard classes and hazard categories	Hazard statements
Flammable liquid, category 2	H225
Aspiration hazard, category 1	H304
Skin irritation, category 2	H315
Specific target organ toxicity (single exposure), category 3, narcotic effect	H336
Hazardous to the aquatic environment, chronic, category 1	H410

2.2 Label elements

2.2.1 Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms



Signal word: Danger

Hazard statements	
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H410	Very 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.
P243	Take precautionary measures against static discharge.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P273	Avoid release to the environment.
P301+P331	IF SWALLOWED: Do NOT induce vomiting.
P302+P352	IF ON SKIN: Wash with plenty of water/...
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P308+P310	IF exposed or concerned: Immediately call a POISON CENTER/doctor.

Other hazards

none



SECTION 3: Composition / information on ingredients

3.1 Substances

Substance name	Isooctane
Molecular formula	(CH ₃) ₂ CHCH ₂ C(CH ₃) ₃
Molecular weight	114.23 g/mol
CAS No.	540-84-1
REACH registration No.	Not yet communicated down the supply chain.
INDEX No.	601-009-00-8

SECTION 4: First aid measures

4.1 General information

IF exposed: Immediately call a POISON CENTRE/doctor. If unconscious place in recovery position and seek medical advice. Never give anything by mouth to an unconscious person or a person with cramps. Change contaminated, saturated clothing. Do not leave affected person unattended.

After inhalation

Immediately call a POISON CENTRE/doctor. Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

In case of skin contact

After contact with skin, wash immediately with plenty of water and soap. Remove contaminated, saturated clothing immediately. In case of skin reactions, consult a physician.

After eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye. Remove contact lenses, if present and easy to do. Continue rinsing.

In case of ingestion

Immediately call a POISON CENTRE/doctor. Do NOT induce vomiting. Rinse mouth thoroughly with water. Give nothing to eat or drink.

4.2 Most important symptoms and effects, both acute and delayed

no data available

4.3 Indication of any immediate medical attention and special treatment needed

no data available

4.4 Self-protection of the first aider

First aider: Pay attention to self-protection!

4.5 Information to physician

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water spray

ABC-powder
Carbon dioxide (CO₂)
Nitrogen

Extinguishing media which must not be used for safety reasons
no restriction

5.2 Special hazards arising from the substance or mixture

In case of fire may be liberated:
Carbon monoxide
Carbon dioxide (CO₂)

5.3 Advice for firefighters

DO NOT fight fire when fire reaches explosives.
Special protective equipment for firefighters
Wear a self-contained breathing apparatus and chemical protective clothing.

Additional information

Do not allow run-off from fire-fighting to enter drains or water courses.
Do not inhale explosion and combustion gases.
Use caution when applying carbon dioxide in confined spaces. Carbon dioxide can displace oxygen.
Use water spray jet to protect personnel and to cool endangered containers.
In case of fire: Evacuate area.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

In case of major fire and large quantities: Remove persons to safety.

6.2 Environmental precautions

Discharge into the environment must be avoided.

6.3 Methods and material for containment and cleaning up

Spilled product must never be returned to the original container for recycling. Collect in closed and suitable containers for disposal.

6.4 Additional information

Clear spills immediately.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid: Inhalation Avoid contact with skin and eyes. Use extractor hood (laboratory). If handled uncovered, arrangements with local exhaust ventilation have to be used. If local exhaust ventilation is not possible or not sufficient, the entire working area must be ventilated by technical means. Keep away from sources of ignition. - No smoking. Usual measures for fire prevention. Take precautionary measures against static discharges.

7.2 Conditions for safe storage, including any incompatibilities

Recommended storage temperature: 15-25°C
Storage class: 3
Keep container tightly closed and in a well-ventilated place. Keep/Store away from combustible materials.



7.3 Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Does not contain substances above concentration limits fixing an occupational exposure limit.

8.2 Exposure controls

8.2.1 Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment. If handled uncovered, arrangements with local exhaust ventilation have to be used.

8.2.2 Personal protection equipment

Wear suitable protective clothing. When handling with chemical substances, protective clothing with CE-labels including the four control digits must be worn.

Eye/face protection

Eye glasses with side protection DIN-/EN-Norms: DIN EN 166

Recommendation: VWR 111-0432

Skin protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. Recommended glove articles DIN-/EN-Norms: DIN EN 374 In the case of wanting to use the gloves again, clean them before taking off and air them well.

By short-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,12 mm
Breakthrough time (maximum wearing time):	> 480 min
Recommended glove articles:	VWR 112-0998

By long-term hand contact

Suitable material:	NBR (Nitrile rubber)
Thickness of the glove material:	0,38 mm
Breakthrough time (maximum wearing time):	> 480 min
Recommended glove articles:	VWR 112-3717 / 112-1381

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

Suitable respiratory protection apparatus:	Full-/half-/quarter-face masks (DIN EN 136/140)
Recommendation:	VWR 111-0206
Suitable material:	ABEK2P3
Recommendation:	VWR 111-0059

Additional information

Wash hands before breaks and after work. Avoid contact with skin and eyes. When using do not eat, drink or smoke. Provide eye shower and label its location conspicuously.

8.2.3 Environmental exposure controls

no data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

(a) Appearance	
Physical state:	liquid
Colour:	colourless
(b) Odour:	no data available
(c) Odour threshold:	no data available

Safety relevant basic data

(d) pH:	7 (20 °C)
(e) Melting point/freezing point:	-107 °C
(f) Initial boiling point and boiling range:	99.2 °C (1013 hPa)
(g) Flash point:	-12 °C
(h) Evaporation rate:	no data available
(i) Flammability (solid, gas):	Highly flammable liquid and vapour.
(j) Flammability or explosive limits	
Lower explosion limit:	1 % (v/v)
Upper explosion limit:	6 % (v/v)
(k) Vapour pressure:	41 mmHg (21 °C)
(l) Vapour density:	3.93 (20 °C)
(m) Relative density:	0.692 g/cm ³ (20 °C)
(n) Solubility(ies)	
Water solubility (g/L):	560 µg/l (25 °C)
Soluble (g/L) in Ethanol:	no data available
(o) Partition coefficient: n-octanol/water:	4.5 (20 °C)
(p) Auto-ignition temperature:	410 °C
(q) Decomposition temperature:	no data available
(r) Viscosity	
Kinematic viscosity:	no data available
Dynamic viscosity:	0.5 mPa*s (20 °C)
(s) Explosive properties:	not applicable
(t) Oxidising properties:	not applicable

9.2 Other information

Bulk density:	not applicable
Refraction index:	1.38962 (589 nm; 20 °C)
Dissociation constant:	no data available
Surface tension:	no data available
Henry constant:	no data available



SECTION 10: Stability and reactivity

10.1 Reactivity

Vapours can form explosive mixtures with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions

Formation of explosive mixtures with:

Oxidising agent, strong

10.4 Conditions to avoid

This material is combustible and can be ignited by heat, sparks, flames, or other sources of ignition (e.g. static electricity, pilot lights, or mechanical/electrical equipment).

10.5 Incompatible materials

Rubber articles

Plastic articles

10.6 Hazardous decomposition products

no data available

10.7 Additional information

no data available

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute effects

Acute oral toxicity:

LD50: < 2500 mg/kg - Rat - (IUCLID)

Acute dermal toxicity:

no data available

Acute inhalation toxicity:

LC50: 47.4 mg/l - Rat - (IUCLID)

Irritant and corrosive effects

Primary irritation to the skin:

Causes skin irritation.

Irritation to eyes:

not applicable

Irritation to respiratory tract:

not applicable

**Respiratory or skin sensitisation**

In case of skin contact: not sensitising

After inhalation: not sensitising

STOT-single exposure

May cause drowsiness or dizziness.

STOT-repeated exposure

not applicable

CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)**Carcinogenicity**

No indication of human carcinogenicity.

Germ cell mutagenicity

No indications of human germ cell mutagenicity exist.

Reproductive toxicity

No indications of human reproductive toxicity exist.

Aspiration hazard

May be fatal if swallowed and enters airways.

Other adverse effects

no data available

Additional information

no data available

SECTION 12: Ecological information

12.1 Ecotoxicity

Fish toxicity:

no data available

Daphnia toxicity:

no data available

Algae toxicity:

no data available

Bacteria toxicity:

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water: 4.5 (20 °C)



12.4 Mobility in soil:

no data available

12.5 Results of PBT/vPvB assessment

no data available

12.6 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Appropriate disposal / Product

Dispose according to local legislation. Consult the appropriate local waste disposal expert about waste disposal.

Waste code product: 070104

Appropriate disposal / Package

Dispose according to local legislation. Handle contaminated packages in the same way as the substance itself.

Additional information

no data available

SECTION 14: Transport information

Land transport (ADR/RID)

14.1	UN-No.:	1262
14.2	Proper Shipping Name:	OCTANES
14.3	Class(es):	3
	Classification code:	F1
	Hazard label(s):	3
14.4	Packing group:	II
14.5	Environmental hazards:	Dangerous for the environment
14.6	Special precautions for user:	
	Hazard identification number (Kemler No.):	33
	tunnel restriction code:	D/E
		(Passage forbidden through tunnels of category D when carried in bulk or in tanks. Passage forbidden through tunnels of category E.)

Sea transport (IMDG)

14.1	UN-No.:	1262
14.2	Proper Shipping Name:	OCTANES
14.3	Class(es):	3
	Classification code:	
	Hazard label(s):	3
14.4	Packing group:	II



SECTION 16: Other information

Abbreviations and acronyms

ACGIH - American Conference of Governmental Industrial Hygienists
ADR - European Agreement concerning the International Carriage of Dangerous Goods by Road
AGS - Committee on Hazardous Substances (Ausschuss für Gefahrstoffe)
CLP - Regulation on Classification, Labelling and Packaging of Substances and Mixtures
DFG - German Research Foundation (Deutsche Forschungsgemeinschaft)
Gestis - Information system on hazardous substances of the German Social Accident Insurance (Gefahrstoffinformationssystem der Deutschen Gesetzlichen Unfallversicherung)
IATA-DGR - International Air Transport Association-Dangerous Goods Regulations
ICAO-TI - International Civil Aviation Organization-Technical Instructions
IMDG - International Maritime Code for Dangerous Goods
LTV - Long Term Value
NIOSH - National Institute for Occupational Safety and Health
OSHA - Occupational Safety & Health Administration
PBT - Persistent, Bioaccumulative and Toxic
RID - Regulation concerning the International Carriage of Dangerous Goods by Rail
STV - Short Term Value
SVHC - Substances of Very High Concern
vPvB - very Persistent, very Bioaccumulative

Additional information

Indication of changes: general update

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.