

# SAFETY DATA SHEET



**NPG Di-heptanoate (CQ) - Cosmetic Quality**  
11990

Version / Revision 1  
Supersedes Version -

Revision Date 15-May-2023  
Issuing date 15-May-2023

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

### 1.1. Product identifier

Identification of the substance/preparation

## NPG Di-heptanoate (CQ) - Cosmetic Quality

Chemical Name Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol  
CAS-No 68855-18-5  
EC No. 272-469-1

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

Use of the Substance / Preparation cosmetics.  
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  
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

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

## SECTION 2: Hazards identification

### Europe

#### 2.1. Classification of the substance or mixture

Based on present data no classification and labelling is required according to Directive 1272/2008/EC and its amendments (CLP Regulation)

#### 2.2. Label elements

Not required.

#### 2.3. Other hazards

If the material is misted or if vapours are generated from heating, exposure may cause irritation of mucous membranes and the upper respiratory tract

**PBT and vPvB assessment** This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

### USA

#### 2.1. Classification of the substance or mixture

This substance is not hazardous in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

**OSHA Specified Hazards** Not applicable.

#### 2.2. Label elements

Not required according to §1910.1200 (GHS-US labeling).

#### 2.3. Other hazards

If the material is misted or if vapours are generated from heating, exposure may cause irritation of mucous membranes and the upper respiratory tract

## SECTION 3: Composition / information on ingredients

### 3.1. Substances

Component	CAS-No	REACH-No	1272/2008/EC	Concentration (%)
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol	68855-18-5	01-2119969496-18	-	> 98

## SECTION 4: First aid measures

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

## 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. Immediate medical attention is required.

### Skin

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

### Ingestion

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

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

### Main symptoms

None known.

### Special hazard

Prolonged skin contact may defat the skin and produce dermatitis.

## 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.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

#### Suitable extinguishing media

foam, dry chemical, carbon dioxide (CO<sub>2</sub>), 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 (CO<sub>2</sub>)

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

Vapours are heavier than air and may spread along floors

### 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.

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

## 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.

## 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).

### 6.3. Methods and material for containment and cleaning up

#### Methods for containment

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. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Dispose of in accordance with local regulations. 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.

#### 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

strong acids  
strong bases  
oxidizing agents

### 7.2. Conditions for safe storage, including any incompatibilities

# SAFETY DATA SHEET



**NPG Di-heptanoate (CQ) - Cosmetic Quality**  
11990

Version / Revision 1

## 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.

## Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care.

## Temperature class

T2

## 7.3. Specific end use(s)

Cosmetics, personal care products

## SECTION 8: Exposure controls / personal protection

### 8.1. Control parameters

#### Exposure limits European Union

No exposure limits established

#### Exposure limits Germany

Under conditions which may generate mists, observe a suggested PEL of 5 mg/m<sup>3</sup> and STEL of 10 mg/m<sup>3</sup>.

#### 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

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

with this chemical, material selection should be based on protection for all chemicals present.

**Suitable material** Neoprene

**Suitable material** nitrile rubber

## Skin and body protection

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

## 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

<b>Appearance</b>	liquid				
<b>Colour</b>	colourless				
<b>Odour</b>	No data available				
<b>Odour threshold</b>	No data available				
<b>pH</b>	No data available				
<b>Melting point/freezing point</b>	-87 °C (Pour point)				
<b>Boiling point or initial boiling point and boiling range</b>	No data available				
<b>Flash point</b>	191 °C				
<b>Method</b>	closed cup, ISO 2719				
<b>Evaporation rate</b>	No data available				
<b>Flammability (solid, gas)</b>	Does not apply, the substance is a liquid				
<b>Lower explosion limit</b>	No data available				
<b>Upper explosion limit</b>	No data available				
<b>Vapour pressure</b>					
Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
<0,01	<0,001	<0,0001	20	68	QSAR
<b>Relative vapour density</b>	No data available				
<b>Density and/or relative density</b>					
Values	@ °C	@ °F	Method		
0,92	20	68	EU A.3		
<b>Solubility</b>	< 0,05 mg/l @ 20 °C, in water, EU A.6				
<b>Partition coefficient n-octanol/water (log value)</b>	6,68 (calculated) KOW WIN				
<b>Autoignition temperature</b>	355 °C				
<b>Method</b>	DIN 51794				
<b>Decomposition temperature</b>	No data available				
<b>Viscosity</b>	10 mm <sup>2</sup> /s @ 20°C				
<b>Oxidizing properties</b>	Does not apply, substance is not oxidising. There are no chemical groups				

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

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

## 9.2. Other information

**Molecular weight** 328,4924  
**Molecular formula** C<sub>19</sub> H<sub>36</sub> O<sub>4</sub>  
**log Koc** 3,69 - 4,49 @ 25°C (77 °F) calculated

## 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 polymerisation does not occur.

### 10.4. Conditions to avoid

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

### 10.5. Incompatible materials

strong acids, strong bases, 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

<b>Acute toxicity</b>				
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	>2000 mg/kg	rat, male/female	OECD 401
Inhalative	LC50	>5,22 mg/l (4h)	rat, male/female	OECD 436

### **Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

#### **Assessment**

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

Acute oral toxicity

Acute inhalation toxicity

# SAFETY DATA SHEET



**NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990**

**Version / Revision 1**

For acute dermal toxicity, no data are available

<b>Irritation and corrosion</b>				
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	not irritating	OECD 404	4h
Eyes	rabbit	Mild eye irritation	OECD 405	

## **Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

### **Assessment**

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

skin irritation/corrosion

eye irritation/corrosion

If the material is misted or if vapours are generated from heating, exposure may cause irritation of mucous membranes and the upper respiratory tract

<b>Sensitization</b>				
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>				
Target Organ Effects	Species	Evaluation	Method	
Skin	guinea pig	not sensitizing	OECD 406	

## **Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

### **Assessment**

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

Skin sensitization

For respiratory sensitization, no data are available

<b>Subacute, subchronic and prolonged toxicity</b>				
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>				
Type	Dose	Species	Method	
Subacute toxicity	NOAEL: $\geq$ 1450 mg/kg/d (28d)	rat, male	OECD 407 Oral	read across
Subchronic toxicity	NOAEL: $\geq$ 1000 mg/kg/d (90d)	rat, male/female	OECD 408 Oral	read across
Subchronic toxicity	NOAEC: 0,5 mg/l/d (13 weeks)	rat, male/female	OECD 413 Inhalation	read across
Subchronic toxicity	NOAEL: $\geq$ 2000 mg/kg/d (13 weeks)	rat, male/female	OECD 411 Dermal	read across

## **Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

### **Assessment**

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

STOT RE

<b>Carcinogenicity, Mutagenicity, Reproductive toxicity</b>					
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	read across
Mutagenicity		human lymphocytes	negative	OECD 473 (Chromosomal Aberration)	
Mutagenicity		mouse	negative	OECD 476	



# SAFETY DATA SHEET



**NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990**

Version / Revision 1

		lymphoma cells		(Mammalian Gene Mutation)	
Developmental Toxicity	NOAEL 2000 mg/kg/d			OECD 414, Dermal	read across systemic effects Maternal toxicity
Developmental Toxicity	NOAEL 200 mg/kg/d			OECD 414, Dermal	read across Local effects Maternal toxicity

## **Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

### **CMR Classification**

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B

### **Evaluation**

In vitro tests did not show mutagenic effects

## **Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

### **Target Organ Systemic Toxicant - Single exposure**

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

### **Target Organ Systemic Toxicant - Repeated exposure**

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

### **Aspiration toxicity**

no data available

### **Note**

Handle in accordance with good industrial hygiene and safety practice.

## **SECTION 12: Ecological information**

### **12.1. Toxicity**

<b>Acute aquatic toxicity</b>			
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>			
Species	Exposure time	Dose	Method
Oncorhynchus mykiss (rainbow trout)	96h	LC50: >0,086 mg/l	OECD 203
Pseudokirchneriella subcapitata	72h	EC50: >0,0065 mg/l (Growth rate)	OECD 201
Activated sludge (domestic)	3 h	NOEC: >=1000 mg/l	OECD 209

<b>Long term toxicity</b>			
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>			
Type	Species	Dose	Method
Reproductive toxicity	Daphnia magna (Water flea)	NOEC: ≥ 0,0019 mg/l	OECD 211
Aquatic toxicity	Pseudokirchneriella subcapitata	NOEC: ≥ 0,0065 mg/l Growth rate	OECD 201

<b>Terrestrial toxicity</b>				
<b>Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)</b>				
Species	Exposure time	Dose	Type	Method
Eisenia fetida	14 d	NOEC: ≥ 1000	Reproduction	OECD 207

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

		mg/kg soil dw		
Eisenia fetida	56 d	NOEC: $\geq$ 1000 mg/kg soil dw	Reproduction	read across OECD 222

## 12.2. Persistence and degradability

Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5

### Biodegradation

89,3 % (28 d), activated sludge (domestic), aerobic, OECD 301 B.

Abiotic Degradation		
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)		
Type	Result	Method
Hydrolysis	5,3 yr@25 °C, pH 7	calculated
Photolysis	Half-life (DT50): 24,32 h	calculated

## 12.3. Bioaccumulative potential

Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)		
Type	Result	Method
BCF	33,76 - 500	QSAR
log Pow	6,68	calculated

## 12.4. Mobility in soil

Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)		
Type	Result	Method
Adsorption/Desorption	Koc: 4929 - 30820	calculated
Surface tension	not applicable	
Distribution to environmental compartments	no data available	

## 12.5. Results of PBT and vPvB assessment

Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5

### PBT and vPvB assessment

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT), nor very persistent nor very bioaccumulating (vPvB)

## 12.6. Other adverse effects

Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5

No data available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Product Information

# SAFETY DATA SHEET



**NPG Di-heptanoate (CQ) - Cosmetic Quality**  
11990

Version / Revision 1

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.

### **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**

### **Section 14.1 - 14.6**

**ICAO-TI / IATA-DGR** Not restricted

**IMDG** Not restricted

**14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code** not applicable

**ADR/RID** Not restricted

## **SECTION 15: Regulatory information**

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

**Regulation 1272/2008, Annex VI** not listed

**DI 2012/18/EU (Seveso III)**  
Category not subject

**DI 1999/13/EC (VOC Guideline)**

Component	Status
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol CAS: 68855-18-5	not subject

### **International Inventories**

**Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol, CAS: 68855-18-5**

AICS (AU)  
NDSL (CA)  
IECSC (CN)  
EC-No. 272-469-1 (EU)  
KECI 2001-3-1721 (KR)  
PICCS (PH)  
TSCA (US)

# SAFETY DATA SHEET



NPG Di-heptanoate (CQ) - Cosmetic Quality  
11990

Version / Revision 1

TCSI (TW)

## SECTION 16: Other information

### 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](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](http://www.chemicals.oq.com)).

The annex is not required because the substance is not classified for human health or the environment, is not a CMR and is not PBT or vPvB

### 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 Chemicals 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.

**End of Safety Data Sheet**