

SAFETY DATA SHEET

according to REACH Regulation (EC) No. 1907/2006, as amended by UK REACH Regulations SI 2019/758



NPG Di-heptanoate (CQ) - Cosmetic Quality
11990

Version / Revision 1
Supersedes Version -

Revision Date 31-Aug-2022
Issuing date 31-Aug-2022

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

Identified uses Cosmetics, personal care products
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

SECTION 2: Hazards identification

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

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

SECTION 3: Composition / information on ingredients

3.1. Substances

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

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.

Skin

Wash off immediately with soap and plenty of water. 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.

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 (CO₂), water spray

Unsuitable Extinguishing Media

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

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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
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.

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

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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

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 UK

No exposure limits established.

DNEL & PNEC

Not required.

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

Workers

DN(M)EL - long-term exposure - systemic effects - Inhalation	No hazard identified
DN(M)EL - acute / short-term exposure - systemic effects - Inhalation	No hazard identified
DN(M)EL - long-term exposure - local effects - Inhalation	No hazard identified
DN(M)EL - acute / short-term exposure - local effects - Inhalation	No hazard identified
DN(M)EL - long-term exposure - systemic effects - Dermal	No hazard identified
DN(M)EL - acute / short-term exposure - systemic effects - Dermal	No hazard identified
DN(M)EL - long-term exposure - local effects - Dermal	No hazard identified

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DN(M)EL - acute / short-term exposure - local effects - Dermal No hazard identified
DN(M)EL - local effects - eyes No hazard identified

General population

DN(M)EL - long-term exposure - systemic effects - Inhalation No hazard identified
DN(M)EL - acute / short-term exposure - systemic effects - Inhalation No hazard identified
DN(M)EL - long-term exposure - local effects - Inhalation No hazard identified
DN(M)EL - acute / short-term exposure - systemic effects - Dermal No hazard identified
DN(M)EL - long-term exposure - local effects - Dermal No hazard identified
DN(M)EL - acute / short-term exposure - local effects - Dermal No hazard identified
DN(M)EL - long-term exposure - systemic effects - Oral No hazard identified
DN(M)EL - acute / short-term exposure - systemic effects - Oral No hazard identified
DN(M)EL - local effects - eyes No hazard identified

Environment

PNEC aqua - freshwater No hazard identified
PNEC aqua - marine water No hazard identified
PNEC aqua - intermittent releases No hazard identified
PNEC STP No hazard identified
PNEC sediment - freshwater No hazard identified
PNEC sediment - marine water No hazard identified
PNEC Air No hazard identified
PNEC soil No hazard identified
Secondary poisoning No potential for bioaccumulation

8.2. Exposure controls

Special adaptations (REACH)

Not applicable.

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.

Equipment should conform to EN 166

Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on

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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 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 organic filter. Full mask with above mentioned filter according to producers using requirements or self-contained breathing apparatus. Equipment should conform to EN 136 or EN 140 and EN 143.

Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emission 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.

Additional advice

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 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	liquid				
Colour	colourless				
Odour	No data available				
Odour threshold	No data available				
pH	No data available				
Melting point/range	-87 °C (Pour point)				
Method	ASTM D 97-02				
Boiling point/range	No data available				
Flash point	191 °C				
Method	closed cup, ISO 2719				
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
<0,01	<0,001	<0,0001	20	68	QSAR
Vapour density	No data available				
Relative density					
Values	@ °C	@ °F	Method		
0,92	20	68	EU A.3		
Solubility	< 0,05 mg/l @ 20 °C, in water, EU A.6				
log Pow	6,68 (calculated) KOW WIN				
Autoignition temperature	355 °C				
Method	DIN 51794				
Decomposition temperature	No data available				

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Viscosity 10 mm²/s @ 20°C
Explosive properties Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties
Oxidizing properties Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties

9.2. Other information

Molecular weight 328,4924
Molecular formula C₁₉ H₃₆ O₄
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

Acute toxicity				
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)				
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:

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Acute oral toxicity
Acute inhalation toxicity
For acute dermal toxicity, no data are available

Irritation and corrosion				
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)				
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

Sensitization				
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)				
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

Subacute, subchronic and prolonged toxicity				
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)				
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

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

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Mutagenicity		mouse lymphoma cells	negative	OECD 476 (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

Acute aquatic toxicity			
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)			
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

Long term toxicity			
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol (68855-18-5)			
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

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

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		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

Disposal required in compliance with all waste management related state and local regulations. The choice of the

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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

ADR/RID

Not restricted

ADN

Not restricted

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

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

The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019 No. 758

Component	Status
Heptanoic acid, ester with 2,2-dimethyl-1,3-propanediol CAS: 68855-18-5	The substance will not be pre-registered

For details and further information please refer to the original regulation.

International Inventories

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

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

National regulatory information Great Britain

Releases to air (Pollution Inventory Substances)

not subject

Releases to water (Pollution Inventory Substances)

not subject

Releases to sewer (Pollution Inventory Substances)

not subject

For details and further information please refer to the original regulation

15.2. Chemical safety assessment

The Chemical Safety Report (CSR) is not required.

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

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 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

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