

### Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878 Issue date: 5/29/2024 Revision date: 12/2/2025 Supersedes version of: 5/29/2024 Version: 2.0

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

#### 1.1. Product identifier

Product form : Substance
Substance name : Musk ketone

IUPAC name : 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone

EC-No. : 201-328-9 CAS-No. : 81-14-1

REACH registration No. : 01-2120766629-37

Product code : 23045
Formula : C14H18N2O5
Product group : Trade product

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

#### Relevant identified uses

Intended for general public

Main use category : Professional use, Consumer use
Use of the substance/mixture : Fragrance raw material

### 1.3. Details of the supplier of the safety data sheet

De Hekserij Spoorstraat 57 8271 RG IJsselmuiden Nederland

T +31 383 557 927

hekserij@hekserij.nl, www.hekserij.nl

### 1.4. Emergency telephone number

No additional information available

# **SECTION 2: Hazards identification**

### 2.1. Classification of the substance or mixture

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

Carcinogenicity, Category 2 H351 Hazardous to the aquatic environment – Acute Hazard, H400

Category 1

Hazardous to the aquatic environment – Chronic Hazard, H410

Category 1

Full text of H- and EUH-statements: see section 16

#### Adverse physicochemical, human health and environmental effects

Suspected of causing cancer. Very toxic to aquatic life with long lasting effects.

### 2.2. Label elements

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

Hazard pictograms (CLP)





GHS08

GHS09

Signal word (CLP) : Warning

Hazard statements (CLP) : H351 - Suspected of causing cancer.

H410 - Very toxic to aquatic life with long lasting effects.

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Precautionary statements (CLP) : P102 - Keep out of reach of children.

P201 - Obtain special instructions before use.

P202 - Do not handle until all safety precautions have been read and understood.

P273 - Avoid release to the environment.

P280 - Wear protective gloves/protective clothing/eye protection/face protection/hearing

rotection.

P308+P313 - IF exposed or concerned: Get medical advice/attention.

P391 - Collect spillage. P405 - Store locked up.

P501 - Dispose of contents and container to hazardous or special waste collection point, in

accordance with local, regional, national and/or international regulation.

#### 2.3. Other hazards

Contains no PBT and/or vPvB substances ≥ 0.1% assessed in accordance with REACH Annex XIII

## **SECTION 3: Composition/information on ingredients**

#### 3.1. Substances

Substance type : Mono-constituent
Name : Musk ketone
CAS-No. : 81-14-1
EC-No. : 201-328-9

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	CAS-No.: 81-14-1 EC-No.: 201-328-9 REACH-no: 01-2120766629- 37	70 – 100	Carc. 2, H351 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Full text of H- and EUH-statements: see section 16

### **SECTION 4: First aid measures**

#### 4.1. Description of first aid measures

First-aid measures general : IF exposed or concerned: Get medical advice/attention.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.

First-aid measures after skin contact : Wash skin with plenty of water.

First-aid measures after eye contact : Rinse eyes with water as a precaution.

First-aid measures after ingestion : Call a poison center or a doctor if you feel unwell.

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

Symptoms/effects after inhalation : Dust of the product, if present, may cause respiratory irritation after excessive inhalation

exposure. Although no appropriate human or animal health effects data are known to exist,

this material is expected to be an inhalation hazard.

Symptoms/effects after skin contact : None under normal conditions. Dust may cause irritation in skin folds or by contact in

combination with tight clothing.

Symptoms/effects after eye contact : None under normal conditions. Dust from this product may cause eye irritation.

Symptoms/effects after ingestion : None under normal conditions.

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

Treat symptomatically.

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### **SECTION 5: Firefighting measures**

### 5.1. Extinguishing media

Suitable extinguishing media : Water spray. Dry powder. Foam. Unsuitable extinguishing media : Do not use a heavy water stream.

#### 5.2. Special hazards arising from the substance or mixture

Fire hazard : No fire hazard.

Explosion hazard : No direct explosion hazard. Hazardous decomposition products in case of fire : Toxic fumes may be released.

#### 5.3. Advice for firefighters

Firefighting instructions : Fight fire from safe distance and protected location. Do not enter fire area without proper

protective equipment, including respiratory protection.

Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained

breathing apparatus. Complete protective clothing.

#### **SECTION 6: Accidental release measures**

#### 6.1. Personal precautions, protective equipment and emergency procedures

General measures : Notify authorities if product enters sewers or public waters. Absorb spillage to prevent

material damage.

For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.

Emergency procedures : Ventilate spillage area.

For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information

refer to section 8: "Exposure controls/personal protection".

Emergency procedures : Evacuate unnecessary personnel.

### 6.2. Environmental precautions

Avoid release to the environment.

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

For containment : Collect spillage.

Methods for cleaning up : Mechanically recover the product. Notify authorities if product enters sewers or public

waters.

Other information : Dispose of materials or solid residues at an authorized site.

#### 6.4. Reference to other sections

For further information refer to section 13.

# **SECTION 7: Handling and storage**

### 7.1. Precautions for safe handling

Additional hazards when processed : Not expected to present a significant hazard under anticipated conditions of normal use.

Precautions for safe handling : Ensure good ventilation of the work station. Obtain special instructions before use. Do not

handle until all safety precautions have been read and understood. Wear personal

protective equipment.

Hygiene measures : Do not eat, drink or smoke when using this product. Always wash hands after handling the

product.

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

Technical measures : Keep in a cool, well-ventilated place away from heat.

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Storage conditions : Store locked up.

Packaging materials : Store always product in container of same material as original container.

## 7.3. Specific end use(s)

No additional information available

### SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

#### **DNEL and PNEC**

Musk ketone (81-14-1)			
DNEL/DMEL (Workers)			
Long-term - systemic effects, dermal	0.563 mg/kg bodyweight/day		
Long-term - systemic effects, inhalation	0.247 mg/m³		
DNEL/DMEL (General population)			
Long-term - systemic effects,oral	25 μg/kg bodyweight/day		
Long-term - systemic effects, inhalation	43.5 μg/m³		
Long-term - systemic effects, dermal	67 μg/kg bodyweight/day		
PNEC (Water)	PNEC (Water)		
PNEC aqua (freshwater)	0.244 μg/l		
PNEC aqua (marine water)	24.4 ng/l		
PNEC aqua (intermittent, freshwater)	2.44 µg/l		
PNEC (Sediment)			
PNEC sediment (freshwater)	61.8 µg/kg dw		
PNEC sediment (marine water)	6.18 µg/kg dw		
PNEC (Soil)			
PNEC soil	12.2 µg/kg dw		
PNEC (STP)			
PNEC sewage treatment plant	10 mg/l		

# 8.2. Exposure controls

#### Appropriate engineering controls

## Appropriate engineering controls:

Ensure good ventilation of the work station.

#### Personal protection equipment

#### Personal protective equipment:

Wear recommended personal protective equipment.

#### Personal protective equipment symbol(s):







### Eye and face protection

### Eye protection:

Safety glasses

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### **Skin protection**

#### Skin and body protection:

Wear suitable protective clothing

### Hand protection:

Protective gloves

#### **Respiratory protection**

#### Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment

#### **Environmental exposure controls**

#### **Environmental exposure controls:**

Avoid release to the environment.

### **SECTION 9: Physical and chemical properties**

#### 9.1. Information on basic physical and chemical properties

Physical state : Solid

Colour : white. light yellow. Odour : Not available Odour threshold : Not available : 135.5 °C Melting point : Not applicable Freezing point Boiling point : Not available Flammability : Non flammable. Lower explosion limit : Not applicable Upper explosion limit : Not applicable Flash point : > 100 °C Auto-ignition temperature : Not applicable : Not available Decomposition temperature : Not available рΗ pH solution : Not available Viscosity, kinematic : Not applicable

Solubility : Insoluble in water. Soluble in ethanol.

Partition coefficient n-octanol/water (Log Kow) : Not available

Vapour pressure : 0.000668 Pa Temp.: 25 °C

Vapour pressure at 50°C : Not available
Density : Not available
Relative density : Not available
Relative vapour density at 20°C : Not applicable
Particle size : Not available

#### 9.2. Other information

No additional information available

### **SECTION 10: Stability and reactivity**

### 10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

#### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

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### 10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).

#### 10.5. Incompatible materials

No additional information available

#### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## **SECTION 11: Toxicological information**

#### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (oral) : Not classified
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Not classified

4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (81-14-1)	
	> 5000 mg/kg bodyweight Animal: rat, Guideline: OECD Guideline 401 (Acute Oral Toxicity)
50 Inhalation - Rat	> 2.99 mg/l air Animal: rat, Guideline: OECD Guideline 403 (Acute Inhalation Toxicity)

 Skin corrosion/irritation
 : Not classified

 Serious eye damage/irritation
 : Not classified

 Respiratory or skin sensitisation
 : Not classified

 Germ cell mutagenicity
 : Not classified

Carcinogenicity : Suspected of causing cancer.

Reproductive toxicity : Not classified STOT-single exposure : Not classified STOT-repeated exposure : Not classified

#### 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (81-14-1)

NOAEL (dermal, rat/rabbit, 90 days)
75 mg/kg bodyweight Animal: rat, Guideline: OECD Guideline 411 (Subchronic Dermal Toxicity: 90-Day Study)

Aspiration hazard : Not classified

### Musk ketone (81-14-1)

Viscosity, kinematic Not applicable

# 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (81-14-1)

Viscosity, kinematic Not applicable

### 11.2. Information on other hazards

No additional information available

# **SECTION 12: Ecological information**

#### 12.1. Toxicity

Ecology - general : Very toxic to aquatic life with long lasting effects.

Hazardous to the aquatic environment, short-term

(acute)

Hazardous to the aquatic environment, long-term : Very toxic to aquatic life with long lasting effects.

(chronic)

### 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (81-14-1)

LC50 - Fish [1] > 0.385 mg/l Test organisms (species): Poecilia reticulata

: Very toxic to aquatic life.

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EC50 - Crustacea [1] > 0.432 mg/l Test organisms (species): Daphnia magna

### 12.2. Persistence and degradability

Musk ketone (81-14-1)		
Persistence and degradability Not rapidly degradable		
4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (81-14-1)		
Persistence and degradability Not rapidly degradable		

### 12.3. Bioaccumulative potential

No additional information available

### 12.4. Mobility in soil

No additional information available

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Endocrine disrupting properties

No additional information available

#### 12.7. Other adverse effects

No additional information available

### **SECTION 13: Disposal considerations**

### 13.1. Waste treatment methods

Regional waste regulation : Disposal must be done according to official regulations.

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.

Sewage disposal recommendations : Disposal must be done according to official regulations.

Product/Packaging disposal recommendations : Comply with applicable regulations for solid waste disposal. Disposal must be done

according to official regulations.

Additional information : Do not re-use empty containers.

### **SECTION 14: Transport information**

In accordance with ADR / IMDG / IATA / ADN / RID

ADR	IMDG	IATA	ADN	RID
14.1. UN number or ID n	14.1. UN number or ID number			
UN 3077	UN 3077	UN 3077	UN 3077	UN 3077
14.2. UN proper shippin	g name			
ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone)	Environmentally hazardous substance, solid, n.o.s. (Musk ketone)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone)

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ADR	IMDG	IATA	ADN	RID
Transport document descr	iption			
UN 3077 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone), 9, III, (-)	UN 3077 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone), 9, III, MARINE POLLUTANT	UN 3077 Environmentally hazardous substance, solid, n.o.s. (Musk ketone), 9, III	UN 3077 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone), 9, III	UN 3077 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Musk ketone), 9, III
14.3. Transport hazard o	class(es)			
9	9	9	9	9
**************************************	**************************************	**************************************	**************************************	9
14.4. Packing group	14.4. Packing group			
III	III	III	III	III
14.5. Environmental hazards				
Dangerous for the environment: Yes	Dangerous for the environment: Yes Marine pollutant: Yes EmS-No. (Fire): F-A EmS-No. (Spillage): S-F	Dangerous for the environment: Yes	Dangerous for the environment: Yes	Dangerous for the environment: Yes
No supplementary information available				

### 14.6. Special precautions for user

#### **Overland transport**

Classification code (ADR) : M7

Special provisions (ADR) : 274, 335, 375, 601

Limited quantities (ADR) : 5kg
Excepted quantities (ADR) : E1

Packing instructions (ADR) : P002, IBC08, LP02, R001

Special packing provisions (ADR) : PP12, B3
Mixed packing provisions (ADR) : MP10

Portable tank and bulk container instructions (ADR) : T1, BK1, BK2, BK3

Portable tank and bulk container special provisions : TP33

(ADR)

Tank code (ADR) : SGAV, LGBV

Vehicle for tank carriage : AT

Transport category (ADR) : 3

Special provisions for carriage - Packages (ADR) : V13

Special provisions for carriage - Bulk (ADR) : VC1, VC2

Special provisions for carriage - Loading, unloading : CV13

and handling (ADR)

Hazard identification number (Kemler No.) : 90

Orange plates :

90 3077

Tunnel restriction code (ADR)

#### Transport by sea

Special provisions (IMDG) : 274, 335, 966, 967, 969

Limited quantities (IMDG) : 5 kg
Excepted quantities (IMDG) : E1
Packing instructions (IMDG) : LP02, P002

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Special packing provisions (IMDG) : PP12
IBC packing instructions (IMDG) : IBC08
IBC special provisions (IMDG) : B3

Tank instructions (IMDG) : BK1, BK2, BK3, T1

Tank special provisions (IMDG) : TP33
Stowage category (IMDG) : A
Stowage and handling (IMDG) : SW23

Air transport

PCA Excepted quantities (IATA) : E1
PCA Limited quantities (IATA) : Y956
PCA limited quantity max net quantity (IATA) : 30kgG
PCA packing instructions (IATA) : 956
PCA max net quantity (IATA) : 400kg
CAO packing instructions (IATA) : 956
CAO max net quantity (IATA) : 400kg

Special provisions (IATA) : A97, A158, A179, A197, A215

ERG code (IATA) : 9L

**Inland waterway transport** 

Classification code (ADN) : M7

Special provisions (ADN) : 274, 335, 375, 601

Limited quantities (ADN) : 5 kg

Excepted quantities (ADN) : E1

Carriage permitted (ADN) : T\* B\*\*

Equipment required (ADN) : PP, A\*\*\*

Number of blue cones/lights (ADN) : 0

Additional requirements/Remarks (ADN) : \* Only in the molten state. \*\* For carriage in bulk see also 7.1.4.1. \*\*\* Only in the case of

transport in bulk.

Rail transport

Classification code (RID) : M7

Special provisions (RID) : 274, 335, 375, 601

Limited quantities (RID) : 5kg
Excepted quantities (RID) : E1

Packing instructions (RID) : P002, IBC08, LP02, R001

Special packing provisions (RID) : PP12, B3
Mixed packing provisions (RID) : MP10

Portable tank and bulk container instructions (RID) : T1, BK1, BK2, BK3

Portable tank and bulk container special provisions : TP33

(RID)

Tank codes for RID tanks (RID) : SGAV, LGBV

Transport category (RID) : 3
Special provisions for carriage – Packages (RID) : W13
Special provisions for carriage – Bulk (RID) : VC1, VC2
Special provisions for carriage - Loading, unloading : CW13, CW31

and handling (RID)

Colis express (express parcels) (RID) : CE11
Hazard identification number (RID) : 90

# 14.7. Maritime transport in bulk according to IMO instruments

Not applicable

### **SECTION 15: Regulatory information**

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

### **EU-Regulations**

### **REACH Annex XVII (Restriction List)**

Not listed on REACH Annex XVII

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#### **REACH Annex XIV (Authorisation List)**

Not listed on REACH Annex XIV (Authorisation List)

#### **REACH Candidate List (SVHC)**

Contains substance(s) listed on the REACH Candidate List < 0.1% or SCL.

### **PIC Regulation (Prior Informed Consent)**

Contains no substance(s) listed on the PIC list (Regulation EU 649/2012 concerning the export and import of hazardous chemicals)

#### **POP Regulation (Persistent Organic Pollutants)**

Contains no substance(s) listed on the POP list (Regulation EU 2019/1021 on persistent organic pollutants)

#### Ozone Regulation (2024/590)

Not listed on the Ozone Depletion list (Regulation EU 2024/590)

#### Council Regulation (EC) for the control of dual-use items

Contains no substance subject to the COUNCIL REGULATION (EC) for the control of dual-use items

#### **Explosives Precursors Regulation (EU 2019/1148)**

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors)

#### **Drug Precursors Regulation (EC 273/2004)**

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances)

### **National regulations**

#### **Netherlands**

SZW-lijst van kankerverwekkende stoffen : The substance is not listed SZW-lijst van mutagene stoffen : The substance is not listed SZW-lijst van reprotoxische stoffen – Borstvoeding : The substance is not listed SZW-lijst van reprotoxische stoffen – : The substance is not listed

Vruchtbaarheid

SZW-lijst van reprotoxische stoffen – Ontwikkeling : The substance is not listed

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out

### **SECTION 16: Other information**

Abbreviations and acronyms:		
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways	
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road	
ATE	Acute Toxicity Estimate	
BCF	Bioconcentration factor	
BLV	Biological limit value	
BOD	Biochemical oxygen demand (BOD)	
COD	Chemical oxygen demand (COD)	
DMEL	Derived Minimal Effect level	
DNEL	Derived-No Effect Level	
EC-No.	European Community number	
EC50	Median effective concentration	
EN	European Standard	
IARC	International Agency for Research on Cancer	

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Abbreviations and acronyms:		
IATA	International Air Transport Association	
IMDG	International Maritime Dangerous Goods	
LC50	Median lethal concentration	
LD50	Median lethal dose	
LOAEL	Lowest Observed Adverse Effect Level	
NOAEC	No-Observed Adverse Effect Concentration	
NOAEL	No-Observed Adverse Effect Level	
NOEC	No-Observed Effect Concentration	
OECD	Organisation for Economic Co-operation and Development	
OEL	Occupational Exposure Limit	
PBT	Persistent Bioaccumulative Toxic	
PNEC	Predicted No-Effect Concentration	
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail	
SDS	Safety Data Sheet	
STP	Sewage treatment plant	
ThOD	Theoretical oxygen demand (ThOD)	
TLM	Median Tolerance Limit	
VOC	Volatile Organic Compounds	
CAS-No.	Chemical Abstract Service number	
N.O.S.	Not Otherwise Specified	
vPvB	Very Persistent and Very Bioaccumulative	
ED	Endocrine disruptor	

Full text of H- and EUH-statements:		
Aquatic Acute 1	Hazardous to the aquatic environment – Acute Hazard, Category 1	
Aquatic Chronic 1	Hazardous to the aquatic environment – Chronic Hazard, Category 1	
Carc. 2	Carcinogenicity, Category 2	
H351	Suspected of causing cancer.	
H400	Very toxic to aquatic life.	
H410	Very toxic to aquatic life with long lasting effects.	

Safety Data Sheet (SDS), EU

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.