SAFETY DATA SHEET

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

n-Undecanal
11270

Version / Revision	5.01	**Revision Date**	27-Jan-2023
Supersedes Version	5.00***	**Issuing date**	27-Jan-2023

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

1.1. Product identifier

Identification of the substance/preparation **n-Undecanal**

CAS-No 112-44-7
EC No. 203-972-6

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

Identified uses Intermediate
Formulation
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

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

Skin corrosion/irritation Category 2, H315
Environmental hazard Aquatic Acute 1; H400
Aquatic Chronic 2; H411
M-Factor: 1 (self-classification)

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 **Warning**

Hazard statements
H315: Causes skin irritation.
H400: Very toxic to aquatic life.
H411: Toxic to aquatic life with long lasting effects.

Precautionary statements
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P273: Avoid release to the environment.
P302 + P352: IF ON SKIN: Wash with plenty of soap and water.
P332 + P313: If skin irritation occurs: Get medical advice/ attention.
P362 + P364: Take off contaminated clothing and wash it before reuse.
P391: Collect spillage.
P501: Dispose of contents/container in accordance with local regulation.

2.3. Other hazards

None known

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

Endocrine disrupting assessments The substance is not listed on the candidate list according to Art. 59(1), REACh. The substance was not assessed as having endocrine disrupting properties according to regulation 2017/2100/EU or 2018/605/EU.

SECTION 3: Composition / information on ingredients

3.1. Substances

Component	CAS-No	1272/2008/EC	Concentration (%)
Undecanal	112-44-7	Skin Irrit. 2; H315 Aquatic Acute 1; H400 Aquatic Chronic 2; H411 M-Factor: 1 (self-classification)	> 90,0

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

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. Obtain medical attention.

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.

Special hazard
Lung oedema.

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
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. 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
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. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. 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

Further info may be available in the appropriate Exposure scenarios in the annex to this SDS.

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.

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.

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.

Temperature class
T4

7.3. Specific end use(s)

Intermediate
Formulation
For specific end use information see the annex of this safety data sheet

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

Undecanal, CAS: 112-44-7

Workers

DN(M)EL - long-term exposure - systemic effects - Inhalation	23,5 mg/m³
DN(M)EL - acute / short-term exposure - systemic effects - Inhalation	No hazard identified
DN(M)EL - long-term exposure - local effects - Inhalation	10 mg/m³
DN(M)EL - acute / short-term exposure - local effects - Inhalation	10 mg/m³
DN(M)EL - long-term exposure - systemic effects - Dermal	3,3 mg/kg bw/day
DN(M)EL - acute / short-term exposure - systemic effects - Dermal	No hazard identified
DN(M)EL - long-term exposure - local effects - Dermal	Low hazard (no threshold derived)
DN(M)EL - acute / short-term exposure - local effects - Dermal	Low hazard (no threshold derived)
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 - 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
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	1,32 µg/l
PNEC aqua - marine water	0,132 µg/l
PNEC aqua - intermittent releases	1,32 µg/l
PNEC STP	24,7 mg/l
PNEC sediment - freshwater	96,9 µg/kg dw
PNEC sediment - marine water	6,69 µg/kg dw
PNEC Air	No hazard identified
PNEC soil	18,61 µg/kg dw
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 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	nitrile rubber
Reference substance	n/i-Undecanal
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,55 mm
Break through time	> 480 min

Suitable material	Viton
Reference substance	n/i-Undecanal
Evaluation	according to EN 374: level 6
Glove thickness	approx 0,5 mm
Break through time	> 480 min

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

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.

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. For specific exposure controls see the annex to this safety data sheet.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	floral
Odour threshold	No data available
Melting point/freezing point	-10 °C (Pour point) @ 1013 hPa
Method	DIN ISO 3016
Boiling point or initial boiling point and boiling range	225 °C @ 1013 hPa
Method	OECD 103
Flammability	Even if not classified as flammable, the product is capable of catching fire or being set on fire.***
Lower explosion limit	No data available
Upper explosion limit	No data available
Flash point	105 °C @ 1013 hPa
Method	ISO 2719
Autoignition temperature	200 °C @ 1014 hPa
Method	DIN 51794
Decomposition temperature	No data available
pH	6,7 (0,012 g/l in water @ 20 °C (68 °F))
Kinematic Viscosity	2,772 mm²/s @ 20 °C
Method	ASTM D445
Solubility	≤ 828,3 g/l @ 20 °C, Octanol
Water solubility	0,012 g/l @ 20 °C, OECD 105
Partition coefficient n-octanol/water (log value)	5,1 @ 25 °C (77 °F) OECD 117

Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
0,38	0,038	< 0,001	20	68	OECD 104
1,4	0,14	0,001	51,4	124,5	OECD 104

Density and/or relative density

Values	@ °C	@ °F	Method
0,828	20	68	DIN 51757

Relative vapour density	5,94 (Air = 1) @ 20 °C (68 °F)
Particle characteristics	not applicable

9.2. Other information

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
Molecular weight	170,29
Molecular formula	C11 H22 O
log Koc	2,84 calculated
Refractive index	1,413 - 1,435 @ 20 °C
Surface tension	44,8 mN/m (0,0115 g/l @ 20°C (68°F)), OECD 115
Evaporation rate	No data available

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 hazard classes as defined in Regulation (EC) No 1272/2008

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

Acute toxicity				
Undecanal (112-44-7)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	> 5000 mg/kg	rat, male/female	OECD 401
Dermal	LD50	> 5000 mg/kg	rabbit	

Undecanal, CAS: 112-44-7
Assessment
Based on available data, the classification criteria are not met for:

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

Irritation and corrosion				
Undecanal (112-44-7)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	irritating	OECD 404	4h read across
Eyes	rabbit	No eye irritation	OECD 405	read across

Undecanal, CAS: 112-44-7
Assessment
The available data lead to the classification given in section 2
Based on available data, the classification criteria are not met for:
eye irritation/corrosion
For respiratory irritation, no data are available

Sensitization				
Undecanal (112-44-7)				
Target Organ Effects	Species	Evaluation	Method	
Skin	Human experience	not sensitizing	Maximisation Test	

Undecanal, CAS: 112-44-7
Assessment
Based on available data, the classification criteria are not met for:
Skin sensitization

Subacute, subchronic and prolonged toxicity				
Undecanal (112-44-7)				
Type	Dose	Species	Method	
Subacute toxicity	NOAEL: 1000 mg/kg/d	rat, male/female	OECD 422	Oral

Undecanal, CAS: 112-44-7
Assessment
Based on available data, the classification criteria are not met for:
STOT RE

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Undecanal (112-44-7)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	In vitro study
Mutagenicity		human lymphocytes	negative	OECD 487	In vitro study
Mutagenicity		V79 cells, Chinese hamster	negative	OECD 476 (Mammalian Gene Mutation)	In vitro study
Reproductive toxicity	NOAEL > 1000 mg/kg/d	rat, parental		OECD 422, Oral	
Reproductive toxicity	NOAEL > 1000 mg/kg/d	rat, 1. Generation, male/female		OECD 422, Oral	

Undecanal, CAS: 112-44-7
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
Did not show reprotoxic effects in animal experiments
In the absence of specific alerts no cancer testing is required

Undecanal, CAS: 112-44-7
Main symptoms
shortness of breath.
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
Due to the viscosity, this product does not present an aspiration hazard

11.2. Information on other hazards

Endocrine disrupting properties
The substance has not been identified as having endocrine disrupting properties in accordance with section 2.3.
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			
Undecanal (112-44-7)			
Species	Exposure time	Dose	Method
Actinopterygii	96h	LC50: 1,97 mg/l	QSAR
Daphnia magna (Water flea)	48h	EC50: 1459 µg/l	OECD 202
Pseudokirchneriella subcapitata	72h	EC50: 132 µg/l	OECD 201 Growth inhibition
Activated sludge (domestic)	3 h	EC50: 85,3 mg/l	OECD 209

Long term toxicity				
Undecanal (112-44-7)				
Type	Species	Dose	Method	
Aquatic toxicity	Pseudokirchneriella subcapitata	NOEC: 23,5 µg/l (3 d) Growth inhibition	OECD 201	

12.2. Persistence and degradability

Undecanal, CAS: 112-44-7
Biodegradation
65 % (28 d), activated sludge (domestic), non-adapted, aerobic, OECD 301 B.

Abiotic Degradation		
Undecanal (112-44-7)		
Type	Result	Method
Hydrolysis	not expected	
Photolysis	No data available	

12.3. Bioaccumulative potential

Undecanal (112-44-7)		
Type	Result	Method
log Pow	5,1 @ 25 °C (77 °F)	OECD 117
BCF	156,6	calculated

12.4. Mobility in soil

Undecanal (112-44-7)		
Type	Result	Method
Surface tension	44,8 mN/m (0,0115 g/l @ 20°C (68°F))	OECD 115
Adsorption/Desorption	log Koc: 2,84	calculated
Distribution to environmental compartments	no data available	

12.5. Results of PBT and vPvB assessment

Undecanal, CAS: 112-44-7
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. Endocrine disrupting properties

The substance has not been identified as having endocrine disrupting properties in accordance with section 2.3.

12.7. Other adverse effects

Undecanal, CAS: 112-44-7
No data available

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

ADR/RID

14.1. UN number or ID number	UN 3082
14.2. UN proper shipping name	Environmentally hazardous substance, liquid, n.o.s. (n-Undecanal)
14.3. Transport hazard class(es)	9
14.4. Packing group	III
14.5. Environmental hazards	Fish and tree
14.6. Special precautions for user	
ADR Tunnel restriction code	(-)
Classification Code	M6
Hazard Number	90

ADN

ADN Container

14.1. UN number or ID number	UN 3082
14.2. UN proper shipping name	Environmentally hazardous substance, liquid, n.o.s. (n-Undecanal)
14.3. Transport hazard class(es)	9
14.4. Packing group	III
14.5. Environmental hazards	Fish and tree
14.6. Special precautions for user	
Classification Code	M6
Hazard Number	90

ICAO-TI / IATA-DGR

14.1. UN number or ID number	UN 3082
14.2. UN proper shipping name	Environmentally hazardous substance, liquid, n.o.s. (n-Undecanal)
14.3. Transport hazard class(es)	9
14.4. Packing group	III
14.5. Environmental hazards	Fish and tree

IMDG

14.1. UN number or ID number	UN 3082
14.2. UN proper shipping name	Environmentally hazardous substance, liquid, n.o.s. (n-Undecanal)
14.3. Transport hazard class(es)	9
14.4. Packing group	III

14.5. Environmental hazards

Marking	Fish and tree
Marine pollutant	yes

14.6. Special precautions for user

EmS	F-A, S-F

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

Regulation 1272/2008, Annex VI
not listed

DI 2012/18/EU (Seveso III)
Category Annex I, part 1:
E1
E2

DI 1999/13/EC (VOC Guideline)

Component	Status
Undecanal CAS: 112-44-7	regulated

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

Component	Status
Undecanal CAS: 112-44-7	The substance will not be pre-registered

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

International Inventories

Undecanal, CAS: 112-44-7
AICS (AU)
DSL (CA)
IECSC (CN)
EC-No. 2039726 (EU)
ENCS (2)-217 (JP)
ENCS (2)-494 (JP)
ISHL (2)-217 (JP)
ISHL (2)-494 (JP)
KECI KE-35050 (KR)
PICCS (PH)
TSCA (US)
NZIoC-NZ with note
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) has been generated. For Exposure Scenarios see the annex.

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3
H315: Causes skin irritation.
H400: Very toxic to aquatic life.
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).

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

Annex to the extended Safety Data Sheet (eSDS)

General information
A quantitative approach used to conclude safe use for:
Long-term Systemic effects via inhalation
Long-term local effects via inhalation
Long-term Systemic effects via skin
Environmental compartment
Assessment tool used:
Chesar 3.5
A qualitative approach used to conclude safe use for:
Long term local hazards via skin
Acute local hazards via skin

Operational conditions and risk management measures
Minimization of manual phases
Work procedures minimizing of splashes and spills
Avoid direct contact with the chemical/the product/the preparation by establishing organisational measures
Supervision in place to check that the RMMs in place are being used correctly and OCs followed.
Good standard of personal hygiene
Wear suitable gloves tested to EN 374 for activities, where direct contact with substance is possible
Full skin coverage with appropriate light-weight barrier material
Wear suitable face shield.

Exposure scenario identification

1 Industrial use resulting in manufacture of another substance (use of intermediates)
2 Formulation & (re)packing of substances and mixtures

Number of the ES 1

Short title of the exposure scenario
Industrial use resulting in manufacture of another substance (use of intermediates)

List of use descriptors

Sector of uses [SU]
SU8: Manufacture of bulk, large scale chemicals (including petroleum products)
SU9: Manufacture of fine chemicals
SU3: Industrial uses: Uses of substances as such or in preparations at industrial sites

Process categories [PROC]
PROC1: Use in closed process, no likelihood of exposure
PROC2: Use in closed, continuous process with occasional controlled exposure
PROC3: Use in closed batch process (synthesis or formulation)
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC15: Use as laboratory reagent

Environmental release categories [ERC]
ERC6a: Industrial use resulting in manufacture of another substance (use of intermediates)

Product characteristics
Refer to attached safety data sheets

Processes and activities covered by the exposure scenario
Use as an intermediate (not related to Strictly Controlled Conditions). Includes incidental exposures during recycling/ recovery, material transfers, storage, sampling, associated laboratory activities, maintenance and loading (ncluding marine vessel/barge, road/rail car and bulk container).

Further explanations
Industrial use
Assumes use at not more than 20°C above ambient temperature (unless stated differently)
Assumes an advanced standard of occupational Health and Safety Management System

Contributing Scenarios

Number of the contributing scenario **1**
Contributing exposure scenario controlling environmental exposure for ERC 6a

Further specification
release factors for (Sp)ERC were modified
Amounts used
Daily amount per site: 5 to
Annual amount per site: 100 to
Fraction of Regional tonnage used locally: 1
Technical conditions and measures at process level (source) to prevent release
Release fraction to air from process: 5%
Release fraction to wastewater from process: 2E-3%%
Release fraction to soil from process: 0.1%
Conditions and measures related to municipal sewage treatment plant
Size of municipal sewage system/ treatment plant (m^3/d): 2000
The minimum grade of elimination in the sewage plant is (%): 73.91
Water flow in sewage/river (m^3/day): 18000

Number of the contributing scenario **2**
Contributing exposure scenario controlling worker exposure for PROC 1

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Assumes use at not more than 20°C above ambient temperature (unless stated differently)
Technical conditions and measures to control dispersion from source towards the worker
Without local exhaust ventilation. provide a basic standard of general ventilation (1 to 3 air changes per hour).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **3**
Contributing exposure scenario controlling worker exposure for PROC 2

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).

Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario 4
Contributing exposure scenario controlling worker exposure for PROC 3

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario 5
Contributing exposure scenario controlling worker exposure for PROC 4

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear chemically resistant gloves (tested to EN374) in combination with 'basic' employee training. Wear respiratory protection (Efficiency: 90 %).

Number of the contributing scenario 6
Contributing exposure scenario controlling worker exposure for PROC 8a

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear chemically resistant gloves (tested to EN374) in combination with 'basic' employee training. Wear respiratory protection (Efficiency: 90 %).

Number of the contributing scenario 7
Contributing exposure scenario controlling worker exposure for PROC 8b

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)

Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 95 % (inhalative).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear chemically resistant gloves (tested to EN374) in combination with 'basic' employee training.

Number of the contributing scenario **8**

Contributing exposure scenario controlling worker exposure for PROC 15

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374. Wear respiratory protection (Efficiency: 90 %).

Exposure estimation and reference to its source

Environment
PEC = predicted environmental concentration (local); RCR = risk characterisation ratio

Fresh Water (Pelagic)	PEC: 1.15E-3 mg/l; RCR: 0.874
Fresh Water (Sediment)	PEC: 0.085 mg/kg dw; RCR: 0.873
Marine Water (Pelagic)	PEC: 1.15E-4 mg/l; RCR: 0.874
Marine Water (Sediment)	PEC: 8.46E-3 mg/kg dw; RCR: 0.873
Agricultural Soil	PEC: 0.011 mg/kg dw; RCR: 0.607
Sewage Treatment Plant (Effluent)	PEC: 0.012 mg/l; RCR: 0.01

Human exposure prediction (oral, dermal, inhalative)
Oral exposure is not expected to occur. Exposure estimates are given for short-term or long-term, systemic or local exposure depending on which lead to more conservative risk characterization ratios. The RMMs described above suffice to control risks for both local and systemic effects.

Proc 1	EE(inhal): 0.284; EE(derm): 0.034
Proc 2	EE(inhal): 2.838; EE(derm): 1.37
Proc 3	EE(inhal): 8.515; EE(derm): 0.69
Proc 4	EE(inhal): 1.419; EE(derm): 0.686
Proc 8a	EE(inhal): 2.838; EE(derm): 1.371
Proc 8b	EE(inhal): 7.095; EE(derm): 1.371
Proc 15	EE(inhal): 1.419; EE(derm): 0.34

Risk characterisation
RCR(inhal): inhalative risk characterisation ratio; RCR(derm): dermal risk characterisation ratio; total RCR= RCR(inhal) +RCR(derm). Where required local and systemic effects were evaluated both for short-term and long-term exposure. The RCR's given correspond in each case to the most conservative calculated values.

Proc 1	RCR(inhal): 0.028; RCR(derm): 0.01
Proc 2	RCR(inhal): 0.284; RCR(derm): 0.415
Proc 3	RCR(inhal): 0.851; RCR(derm): 0.209
Proc 4	RCR(inhal): 0.142; RCR(derm): 0.208

Proc 8a	RCR(inhal): 0.284; RCR(derm): 0.415
Proc 8b	RCR(inhal): 0.71; RCR(derm): 0.415
Proc 15	RCR(inhal): 0.142; RCR(derm): 0.103

Number of the ES 2

Short title of the exposure scenario

Formulation & (re)packing of substances and mixtures

Sector of uses [SU]

SU3: Industrial uses: Uses of substances as such or in preparations at industrial sites
SU10: Formulation [mixing] of preparations and/or re-packaging (excluding alloys)

Process categories [PROC]

PROC1: Use in closed process, no likelihood of exposure
PROC2: Use in closed, continuous process with occasional controlled exposure
PROC3: Use in closed batch process (synthesis or formulation)
PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises
PROC5: Mixing or blending in batch processes for formulation of preparations and articles (multistage and/or significant contact)
PROC8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities
PROC8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
PROC9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC15: Use as laboratory reagent

Environmental release categories [ERC]

ERC2: Formulation of preparations (mixtures)

Processes and activities covered by the exposure scenario

Formulation, packing and re-packing of the substance and its mixtures in batch or continuous operations, including storage, materials transfers, mixing, tabletting, compression, pelletisation, extrusion, large and small scale packing, sampling, maintenanance and associated laboratory activities.

Further explanations

Industrial use
Assumes use at not more than 20°C above ambient temperature (unless stated differently)
Assumes an advanced standard of occupational Health and Safety Management System

Number of the contributing scenario 1
Contributing exposure scenario controlling environmental exposure for ERC 2

Further specification
release factors for (Sp)ERC were modified.
Amounts used
Daily amount per site: 1 to
Annual amount per site: 100 to
Fraction of Regional tonnage used locally: 1
Technical conditions and measures at process level (source) to prevent release
Release fraction to air from process: 2.5%
Release fraction to wastewater from process: 0.01%
Release fraction to soil from process: 0.01%
Conditions and measures related to municipal sewage treatment plant
Size of municipal sewage system/ treatment plant (m^3/d): 2000
Water flow in sewage/river (m^3/day): 18000
The minimum grade of elimination in the sewage plant is (%): 76,91

Number of the contributing scenario 2
Contributing exposure scenario controlling worker exposure for PROC 1

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor and outdoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Without local exhaust ventilation.
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario 3
Contributing exposure scenario controlling worker exposure for PROC 2

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario 4
Contributing exposure scenario controlling worker exposure for PROC 3

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario 5
Contributing exposure scenario controlling worker exposure for PROC 4

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374. Wear respiratory protection (Efficiency: 90 %).

Number of the contributing scenario **5**
Contributing exposure scenario controlling worker exposure for PROC 5

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear chemically resistant gloves (tested to EN374) in combination with 'basic' employee training. Wear respiratory protection (Efficiency: 90 %).

Number of the contributing scenario **6**
Contributing exposure scenario controlling worker exposure for PROC 8a

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear chemically resistant gloves (tested to EN374) in combination with 'basic' employee training. Wear respiratory protection (Efficiency: 90 %).

Number of the contributing scenario **7**
Contributing exposure scenario controlling worker exposure for PROC 8b

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 95 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374.

Number of the contributing scenario **8**
Contributing exposure scenario controlling worker exposure for PROC 9

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure

Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374. Wear respiratory protection (Efficiency: 90 %).

Number of the contributing scenario **9**

Contributing exposure scenario controlling worker exposure for PROC 15

Product characteristics
Covers percentage substance in the product up to 100 % (unless stated differently)
Liquid
Frequency and duration of use
8 h (full shift)
Other given operational conditions affecting workers exposure
Indoor use
Technical conditions and measures to control dispersion from source towards the worker
provide a basic standard of general ventilation (1 to 3 air changes per hour). Effectiveness of LEV (local exhaust ventilation): 90 % (inhalative); 0 % (dermal).
Conditions and measures related to personal protection, hygiene and health evaluation
Wear suitable gloves tested to EN374. Wear respiratory protection (Efficiency: 90 %).

Environment
PEC = predicted environmental concentration (local); RCR = risk characterisation ratio

Fresh Water (Pelagic)	PEC: 1.15E-3 mg/l; RCR: 0.874
Fresh Water (Sediment)	PEC: 0.085 mg/kg dw; RCR: 0.873
Marine Water (Pelagic)	PEC: 1.15E-4 mg/l; RCR: 0.874
Marine Water (Sediment)	PEC: 8.46E-3 mg/kg dw; RCR: 0.873
Agricultural Soil	PEC: 0.011 mg/kg dw; RCR: 0.585
Sewage Treatment Plant (Effluent)	PEC: 0.012 mg/l; RCR: 0.01

Human exposure prediction (oral, dermal, inhalative)
Oral exposure is not expected to occur. The RMMs described above suffice to control risks for both local and systemic effects. EE(inhal): Estimated inhalative exposure [mg/m³]. EE(derm): Estimated dermal exposure [mg/kg b.w./d]. Exposure estimates are given for short-term or long-term, systemic or local exposure depending on which lead to more conservative risk characterization ratios.

Proc 1	EE(inhal): 0.284; EE(derm): 0.034
Proc 2	EE(inhal): 2.838; EE(derm): 1.37
Proc 3	EE(inhal): 8.515; EE(derm): 0.138
Proc 4	EE(inhal): 1.419; EE(derm): 1.372
Proc 5	EE(inhal): 1.419; EE(derm): 1.371
Proc 8a	EE(inhal): 2.838; EE(derm): 1.371
Proc 8b	EE(inhal): 7.095; EE(derm): 2.742
Proc 9	EE(inhal): 1.419; EE(derm): 1.372
Proc 15	EE(inhal): 1.419; EE(derm): 0.34

Risk characterisation
RCR(inhal): inhalative risk characterisation ratio; RCR(derm): dermal risk characterisation ratio; total RCR= RCR(inhal) +RCR(derm). Where required local and systemic effects were evaluated both for short-term and long-term exposure. The RCR's given correspond in each case to the most conservative calculated values.

Proc 1	RCR(inhal): 0.028; RCR(derm): 0.01
Proc 2	RCR(inhal): 0.284; RCR(derm): 0.415
Proc 3	RCR(inhal): 0.851; RCR(derm): 0.042
Proc 4	RCR(inhal): 0.142; RCR(derm): 0.416
Proc 5	RCR(inhal): 0.142; RCR(derm): 0.415

Proc 8a	RCR(inhal): 0.284; RCR(derm): 0.415
Proc 8b	RCR(inhal): 0.71; RCR(derm): 0.831
Proc 9	RCR(inhal): 0.142; RCR(derm): 0.416
Proc 15	RCR(inhal): 0.142; RCR(derm): 0.103

Guidance to Downstream User to evaluate whether he works inside the boundaries set by the ES
Usage of relase factors allows downstream users to verify in a first approximation, if the combination of local usage and production conditions meets the defined release quantities resulting from this exposure scenario (calculated as M(site) [see amounts used, contributing scenario 1] x release factor [Technical conditions and measures at process level (source) to prevent release; contributing scenario 1])
For specific information regarding the SPERC used please refer to the ESIG webpage https://www.esig.org/reach-ges/environment/

associated uses:

Other combinations of operational conditions may also be safe. Please contact OQ in case your local operational conditions differ from the ones described above and you are unsure if they are also safe