

according to Regulation (EU) nr. 1907/2006

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Product name Isoretinol acetate

Product code 04 0591 4

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

Use - intermediate in the isotretinoin (Roaccutan) synthesis

1.3. Details of the supplier of the safety data sheet

Company information	Enquiries:	Local representation:
	F. Hoffmann-La Roche AG	
	Postfach	
	CH-4070 Basel	
	Switzerland	
	Phone	+41-61/688 54 80
	Fax	+41-61/681 72 76
	E-Mail	info.sds@roche.com

1.4. Emergency telephone number

Emergency telephone number Phone +41-61/688 54 80

SECTION 2: Hazards identification

2.1. / 2.2. Classification of the substance or mixture / Label elements

GHS Classification

Health Hazards:

- 3.2 Skin corrosion/irritation (Category 2)
H315 Causes skin irritation.
- 3.3 Serious eye damage/eye irritation (Category 2A)
H319 Causes serious eye irritation.
- 3.7 Reproductive toxicity (Category 1A)
H360D May damage the unborn child.
- 3.8 Specific target organ toxicity - Single exposure (Category 3)
H335 May cause respiratory irritation.

Environmental Hazards:

- 4.1 Hazardous to the aquatic environment (Category 3)
H412 Harmful to aquatic life with long lasting effects.

Signalword: Danger

Label:



Precautionary statements:

- P201 Obtain special instructions before use.
- P273 Avoid release to the environment.
- P281 Use personal protective equipment as required.
- P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P312 Call a POISON CENTER or doctor/physician if you feel unwell.

2.3. Other hazards

Note

- Women of childbearing potential must not be engaged in any work where dust exposure might occur. In case of doubt a risk assessment is advised.

SECTION 3: Composition/information on ingredients

Characterization

intermediate from the group of retinoids

Chemical name

- 3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-cis,4,6,8-nonatetraenyl acetate

Synonyms

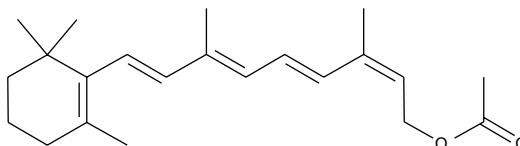
- 13-cis-retinyl acetate
- (2Z,4E,6E,8E)-3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraenyl acetate
- (13Z)-retinyl acetate
- 13-cis vitamin A acetate

CAS number

34356-31-5

Isoretinol acetate

EINECS number	251-956-2
Roche number	Ro0117627-000
Empirical formula	C ₂₂ H ₃₂ O ₂
Molecular mass	328.49 g/mol



SECTION 4: First aid measures

4.1. Description of first aid measures

Eye contact	<ul style="list-style-type: none">- rinse immediately with tap water for 10 minutes - open eyelids forcibly- consult a physician
Skin contact	<ul style="list-style-type: none">- remove immediately contaminated clothes, wash affected skin with water and soap - do not use any solvents- consult physician
Inhalation	<ul style="list-style-type: none">- remove the casualty to fresh air and keep him/her calm- get medical treatment

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

Note	<ul style="list-style-type: none">- no information available
------	--

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

Note to physician	<ul style="list-style-type: none">- treat symptomatically- after accidental exposure women should get medical advice from a physician
-------------------	--

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	<ul style="list-style-type: none">- foam, powder, carbon dioxide
Unsuitable extinguishing media	<ul style="list-style-type: none">- use water spray for cooling purposes only (fat explosion hazard)

5.2. Special hazards arising from the substance or mixture

Specific hazards	<ul style="list-style-type: none">- heating of container(s) will cause pressure rise with risk of bursting and subsequent explosion
------------------	---

5.3. Advice for firefighters

- | | |
|---------------------------------|---|
| Protection of fire-fighters | - precipitate gases/vapours/mists with water spray |
| Special method of fire-fighting | - cool endangered containers with water spray
- remove undamaged containers from heat radiation
- for reasons of environmental protection hold the extinguishing agent back |

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

- | | |
|----------------------|------------------------|
| Personal precautions | - prevent any exposure |
|----------------------|------------------------|

6.2. Environmental precautions

- | | |
|--------------------------|---|
| Environmental protection | - if possible close leaks
- collect the leaked product by all means available
- if the substance reaches waters or the sewer system, inform the competent authority |
|--------------------------|---|

6.3. Methods and material for containment and cleaning up

- | | |
|-------------------------|--|
| Methods for cleaning up | - collect spills with inert adsorbent and hand over to waste removal
- clean contaminated areas with little ethanol |
|-------------------------|--|

SECTION 7: Handling and storage

7.1. Precautions for safe handling

- | | |
|--------------------|--|
| Technical measures | - processing in closed systems, superposed by inert gas (e.g. nitrogen)
- local exhaust ventilation necessary
- take precautionary measures against electrostatic charging |
| Suitable materials | - stainless steel, aluminium, enamel, glass, polyethylene |

7.2. Conditions for safe storage, including any incompatibilities

- | | |
|---------------------|---|
| Storage conditions | - store under inert gas
- store in a dry place
- cool
- protected from light |
| Validity | - 6 months, 5 °C |
| Packaging materials | - tightly closing; material: dark glass, stainless steel, aluminium |

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Threshold value (Roche) air - IOEL (Internal Occupational Exposure Limit): 0.004 mg/m³ *1

8.2. Exposure controls

General protective and hygiene measures - instruction of employees mandatory

Respiratory protection - respiratory protection not necessary during normal operations
- in case of intense formation of aerosols: respirator with independent air supply or particle respectively filter mask (depending on the aerosol composition)

Hand protection - protective gloves (eg made of neoprene, nitrile or butyl rubber)

Eye protection - safety glasses

Body protection - protective clothing

*1 referring to: Tretinoin

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Colour slightly yellowish
Form liquid, viscous
Solubility insoluble, water
soluble, ethanol
well soluble, lipophilic solvents

9.2. Other information

Note - may contain hexane (< 5%) and all-trans-retinol acetate (< 2%) as impurities

General physical and chemical properties

Purity > 94 %

SECTION 10: Stability and reactivity

10.1. Reactivity

Note - no information available

Isoretinol acetate

10.2. Chemical stability

Note - no information available

10.3. Possibility of hazardous reactions

Note - no information available

10.4. Conditions to avoid

Conditions to avoid - light (gradual decomposition)
- warming (gradual decomposition)

10.5. Incompatible materials

Materials to avoid - acids, oxidizing agents, bases
- oxygen in any form especially in the presence of light and/or heat

10.6. Hazardous decomposition products

Note - autooxidation in the presence of air

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity	- LD ₅₀	2'000	mg/kg	(oral, rat)	*1
	- LD ₅₀	2'200	mg/kg	(oral, mouse)	*1
Local effects	-	strong skin irritation, may be increased by UV light			*1
	-	eye: irritant			*1
	-	mucous membranes: irritant			*1
Reproductive toxicity	-	teratogenic (in-vitro assay)			
	-	teratogenic (man); teratogenic in experimental animals at doses > 0.5 mg/kg/day (oral, s.c., rabbit)			*1
Note	-	isoretinol acetate is per se probably significantly less teratogenic and less irritating to skin and mucous membranes than tretinoin; when released into the environment, however, isoretinol acetate is easily oxidized to retinoic acid, hence the stricter precautions regarding tretinoin should apply			

*1 referring to: Tretinoin

SECTION 12: Ecological information

12.1. Toxicity

- Ecotoxicity
- moderately toxic for fish (rainbow trout)
LC₅₀ (96 h) 10.5 mg/l
LC₁₀₀ (96 h) 19.5 mg/l
NOEC (96 h) < 7.6 mg/l
LC₀ (96 h) 7.6 mg/l
(OECD No. 203, tested with the aid of solubilizers)

12.2. Persistence and degradability

- Inherent biodegradability
- well inherently biodegradable
75 %, 28 days
(MITI Test II, OECD No. 302 C)

12.3. Bioaccumulative potential

- Note
- no information available

12.4. Mobility in soil

- Note
- no information available

12.5. Results of PBT and vPvB assessment

- Note
- no information available

12.6. Other adverse effects

- Air pollution
- observe local/national regulations

SECTION 13: Disposal considerations

13.1. Waste treatment methods

- Waste from residues
- incinerate in qualified installation with flue gas scrubbing
 - observe local/national regulations regarding waste disposal

SECTION 14: Transport information

- Note
- not classified by transport regulations

SECTION 15: Regulatory information

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

Water hazard class (Germany)	2: hazardous for water (own classification according to directive VwVwS of 27.07.2005)
------------------------------	--

SECTION 16: Other information

Safety-lab number	- BS-1847
-------------------	-----------

Edition documentation	- changes from previous version in sections 2
-----------------------	---

The information in this safety data sheet is based on current scientific knowledge. It should not be taken as expressing or implying any warranty concerning product characteristics.