

Safety Data Sheet**Ibandronat I**

according to Regulation (EU) nr. 453/2010

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

Product name	Ibandronat I
Product code	04 7912 8

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

Use	- intermediate in the synthesis of an active pharmaceutical compound
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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
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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 1)
H318 Causes serious eye damage.
- 3.4 Skin sensitization (Category 1)
H317 May cause an allergic skin reaction.

Signalword: Danger

Label:



Precautionary statements:

- P280 Wear protective gloves/ protective clothing / eye protection / face protection.
- 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.
- P261 Avoid breathing vapour

2.3. Other hazards

Note

- no information available

SECTION 3: Composition/information on ingredients

Chemical name - N-(Phenylmethylene)-1-pentanamine

Synonyms

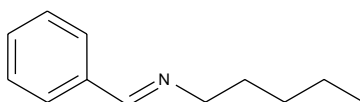
- BM 91.0040
- N-Benzylidene-N-pentylamine
- Ibandron acid step I

CAS number 22710-00-5

Roche number RO0833750-000

Empirical formula $C_{12}H_{17}N$

Molecular mass 175.28 g/mol



SECTION 4: First aid measures

4.1. Description of first aid measures

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|--------------|---|
| Eye contact | - rinse immediately with tap water for 10 minutes - open eyelids forcibly |
| Skin contact | - remove immediately contaminated clothes, wash affected skin with water and soap - do not use any solvents |
| Inhalation | - remove the casualty to fresh air and keep him/her calm |

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

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|------|----------------------------|
| Note | - no information available |
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4.3. Indication of any immediate medical attention and special treatment needed

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|-------------------|-------------------------|
| Note to physician | - treat symptomatically |
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SECTION 5: Firefighting measures

5.1. Extinguishing media

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| Suitable extinguishing media | - water spray jet, dry powder, foam, carbon dioxide |
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5.2. Special hazards arising from the substance or mixture

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| Specific hazards | - formation of toxic and corrosive combustion gases (nitrogen oxides (NO _x)) possible
- heating of container(s) will cause pressure rise with risk of bursting and subsequent explosion |
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5.3. Advice for firefighters

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| Protection of fire-fighters | - precipitate gases/vapours/mists with water spray
- use self-contained breathing apparatus |
| Special method of fire-fighting | - cool endangered containers with water spray |

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

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|----------------------|---|
| Personal precautions | - if this is not endangering the action force or other people, ventilate sewers and cellars |
|----------------------|---|

6.2. Environmental precautions

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|--------------------------|---|
| Environmental protection | <ul style="list-style-type: none">- if possible close leaks- if the substance reaches waters or the sewer system, inform the competent authority |
|--------------------------|---|

6.3. Methods and material for containment and cleaning up

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|-------------------------|---|
| Methods for cleaning up | <ul style="list-style-type: none">- collect liquid by means of sand, earth or another suitable material or cover it with alcohol-resistant foam- during the pouring by a pump bear in mind adequate earthing- collect the product spilled out into ventilated containers equipped with absorption filters |
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SECTION 7: Handling and storage

7.1. Precautions for safe handling

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|--------------------|--|
| Technical measures | <ul style="list-style-type: none">- processing in closed systems, if possible superposed by inert gas (e.g. nitrogen)- local exhaust ventilation necessary- take precautionary measures against electrostatic charging |
| Suitable materials | <ul style="list-style-type: none">- aluminium, enamel, stainless steel |

7.2. Conditions for safe storage, including any incompatibilities

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|---------------------|---|
| Storage conditions | <ul style="list-style-type: none">- dry, cool and ventilated place- secure container and keep tightly closed |
| Packaging materials | <ul style="list-style-type: none">- tightly closing; material: aluminium, stainless steel |

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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|------|--|
| Note | <ul style="list-style-type: none">- no information available |
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8.2. Exposure controls

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|---|---|
| General protective and hygiene measures | <ul style="list-style-type: none">- cleanse skin thoroughly after work, apply skin cream |
| Respiratory protection | <ul style="list-style-type: none">- in case of open handling or accidental release: protective mask with combination filter (e.g. ABEKP) or special filter (e.g. BEP) or respirator with independent air supply |
| Hand protection | <ul style="list-style-type: none">- protective gloves (eg made of NBR Acrylnitril-Butadien-Rubber) |
| Eye protection | <ul style="list-style-type: none">- safety glasses (i.e. in capsule-shaped frames) |

Body protection	- disposable (eg TYVEK) or reusable protective clothing; the latter must be washed (decontaminated) after use
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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Colour	light yellow
Form	liquid
Solubility	280 mg/l, water (20 °C, OECD No. 105)
Partition coefficient	log P _{ow} 2.24 (octanol/water) (Shake Flask Method, OECD No. 107)
Melting temperature	< -77 °C (OECD No. 102)
Boiling temperature	250.2 °C (99 kPa) (OECD No. 103)
Vapour pressure	0.9 Pa (15 °C) 2.3 Pa (25 °C) 4.5 Pa (35 °C) (OECD No. 104)
Flash point (liquid)	109.7 °C (DIN 51'755)
Ignition point (liquid)	250 °C

9.2. Other information

Note	- non-explosive (Expert Statement)
Surface tension	62.1 mN/m (19.3 °C) (OECD No. 115, "Surface Tension of Aqueous Solutions")

SECTION 10: Stability and reactivity

10.1. Reactivity

Note	- no information available
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10.2. Chemical stability

Stability	- stable under the conditions mentioned in chapter 7
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10.3. Possibility of hazardous reactions

Note	- no information available
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10.4. Conditions to avoid

Note - no information available

10.5. Incompatible materials

Note - no information available

10.6. Hazardous decomposition products

Note - no information available

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - LD₅₀ > 2'000 mg/kg (oral, rat)

Local effects - skin: irritant
- eye: irritant; expert statement

Sensitization - sensitizing (mouse)
(OECD No. 429, LLNA (Local Lymph Node Assay))

Mutagenicity - not mutagenic (various in vitro test systems)

SECTION 12: Ecological information

12.1. Toxicity

Ecotoxicity - moderately toxic for planktonic crustaceans (*Daphnia magna*)
EC₅₀ (48 h) 31.7 mg/l
NOEC (48 h) 17.6 mg/l
(OECD No. 202)

12.2. Persistence and degradability

Ready biodegradability - readily biodegradable
98 %, 7 d
(DOC Die-Away Test, OECD No. 301A)

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

PBT/vPvB - not PBT, not vPvB

12.6. Other adverse effects

Air pollution - observe local/national regulations

SECTION 13: Disposal considerations

13.1. Waste treatment methods

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

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) 1: weakly hazardous for water (own classification according to directive VwVwS of 17.05.1999)

SECTION 16: Other information

Safety-lab number - BS-7967

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.