

Safety Data Sheet**PTH-Aminoalcohol**

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 PTH-Aminoalcohol

Product code 04 2979 1

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

Use - intermediate in the HIV-protease inhibitor synthesis

1.3. Details of the supplier of the safety data sheet

Company information

Enquiries:
F. Hoffmann-La Roche AG
Postfach
CH-4070 Basel
Switzerland

Local representation:

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:

- 3.1 Acute toxicity (Category 4)
- H302 Harmful if swallowed.

Environmental Hazards:

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

Signalword: Warning

Label:



Precautionary statements:

- P273 Avoid release to the environment.
- P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.

2.3. Other hazards

Note

- may form explosible dust-air mixture if dispersed

SECTION 3: Composition/information on ingredients

Chemical name

- 2-[3(S)-Amino-2(R)-hydroxy-4-phenylbutyl]-N-tert-butyl-decahydro-(4aS,8aS)-isoquinoline-3(S)-carboxamide

Synonyms

- PTH-AA

CAS number

136522-17-3

Roche number

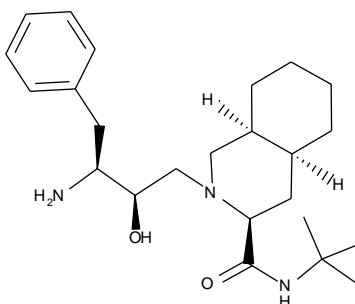
Ro0319232-000

Empirical formula

C₂₄H₃₉N₃O₂

Molecular mass

401.60 g/mol



SECTION 4: First aid measures

4.1. Description of first aid measures

- | | |
|--------------|---|
| Eye contact | - rinse immediately with tap water for at least 20 minutes - open eyelids forcibly |
| Skin contact | - remove immediately contaminated clothes, wash affected skin with plenty of water
- consult a physician if skin irritation persists |
| Inhalation | - remove the casualty to fresh air and keep him/her calm
- in the event of symptoms get medical treatment |

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

- | | |
|------|----------------------------|
| Note | - no information available |
|------|----------------------------|

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

- | | |
|-------------------|-------------------------|
| Note to physician | - treat symptomatically |
|-------------------|-------------------------|

SECTION 5: Firefighting measures

5.1. Extinguishing media

- | | |
|------------------------------|---|
| Suitable extinguishing media | - water spray jet, dry powder, foam, carbon dioxide |
|------------------------------|---|

5.2. Special hazards arising from the substance or mixture

- | | |
|------------------|---|
| Specific hazards | - formation of toxic and corrosive combustion gases (ammonia, hydrogen cyanide, nitrogen oxides) possible
- consider dust explosion hazard |
|------------------|---|

5.3. Advice for firefighters

- | | |
|-----------------------------|--|
| Protection of fire-fighters | - precipitate gases/vapours/mists with water spray |
|-----------------------------|--|

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

- | | |
|----------------------|-------------------------------|
| Personal precautions | - ensure adequate ventilation |
|----------------------|-------------------------------|

6.2. Environmental precautions

Environmental protection	<ul style="list-style-type: none">- dilute the leaked substance by a water spray jet as far as necessary in order to minimize the hazard; hold the draining water/mixture of substances back by all means available- do not allow to enter drains or waterways- 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	<ul style="list-style-type: none">- collect solids (avoid dust formation) and hand over to waste removal
-------------------------	--

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Technical measures	<ul style="list-style-type: none">- processing in closed systems, superposed by inert gas (e.g. nitrogen)- local exhaust ventilation necessary- take precautionary measures against electrostatic charging- avoid dust formation; very high dust explosion hazard
Suitable materials	<ul style="list-style-type: none">- stainless steel, polyethylene

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions	<ul style="list-style-type: none">- room temperature
Validity	<ul style="list-style-type: none">- 12 months, 15 to 25 °C
Packaging materials	<ul style="list-style-type: none">- tightly closing; material: stainless steel (lined with polyethylene bag)

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Threshold value (Roche) air	<ul style="list-style-type: none">- IOEL (Internal Occupational Exposure Limit): 1 mg/m³
-----------------------------	---

8.2. Exposure controls

Respiratory protection	<ul style="list-style-type: none">- in case of open handling or accidental release: particle mask or respirator with independent air supply
Hand protection	<ul style="list-style-type: none">- protective gloves (eg made of neoprene, nitrile or butyl rubber)
Eye protection	<ul style="list-style-type: none">- safety glasses
Analytics	<ul style="list-style-type: none">- sampling on teflon filters through IOM cassette and quantified by an HPLC-UV method

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Colour	white to yellowish
Form	crystalline powder
Odour	odourless
Density	1.136 g/cm ³ (20 °C; OECD No. 109)
Solubility	20'000 mg/l, ethanol (25 °C) 210'000 mg/l, ethanol (78 °C) 21.6 mg/l, water (20 °C, OECD No. 105)
Partition coefficient	log P _{ow} 2.5 (n-octanol/water 23 °C) pH 5.5 (Shake Flask Method, OECD No. 107)
Melting temperature	172.1 °C (OECD No. 102)
Boiling temperature	> 220 °C (970 hPa) (OECD No. 103) decomposes without clearly defined boiling point
Vapour pressure	< 1 Pa (25 °C) (OECD No. 104)

9.2. Other information

Note - no information available

SECTION 10: Stability and reactivity

10.1. Reactivity

Note - no information available

10.2. Chemical stability

Stability - stable under the conditions mentioned in chapter 7

10.3. Possibility of hazardous reactions

Note - no information available

10.4. Conditions to avoid

Note - no information available

10.5. Incompatible materials

Materials to avoid - acids

10.6. Hazardous decomposition products

Note - no information available

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity	<ul style="list-style-type: none"> - LD₅₀ > 500 mg/kg (oral, rat) - LD₅₀ > 2'000 mg/kg (dermal, rat) (OECD No. 402)
Subchronic toxicity	- NOEL 45 mg/kg/d (oral, rat; 28 days)
Local effects	<ul style="list-style-type: none"> - eye: non-irritant (rabbit; OECD No. 405) - skin: non-irritant (rabbit; OECD No. 404)
Sensitization	- non-sensitizing (guinea pig) (OECD No. 406)
Mutagenicity	- not mutagenic (various in vitro test systems)
Carcinogenicity	- no information available
Reproductive toxicity	- no information available
STOT-single exposure	- no information available
STOT-repeated exposure	- no information available
Aspiration hazard	- no information available
Note	- no toxic effects have been observed during occupational handling

SECTION 12: Ecological information

12.1. Toxicity

Ecotoxicity	<ul style="list-style-type: none"> - moderately toxic for algae (<i>Scenedesmus</i> (=Desmodesmus) subspicatus) NOEC (72 hours) 2.47 mg/l LOEC (72 hours) 8.22 mg/l EbC₅₀ (72 hours) 12.7 mg/l (OECD No. 201) - moderately toxic for planktonic crustaceans (<i>Daphnia magna</i>) EC₅₀ (48 hours) 20.1 mg/l NOEC (48 hours) 2.84 mg/l (OECD No. 202) - water soluble part barely toxic for fish (zebrafish) NOEC (96 hours) ≥ 30.2 mg/l (OECD No. 202)
-------------	--

PTH-Aminoalcohol

- activated sludge
NOEC (3 h) < 10 mg/l
EC₂₀ (3 h) 11 mg/l
EC₅₀ (3 h) > 1000 mg/l (nominal concentration)
(OECD No. 209)

12.2. Persistence and degradability

- | | |
|---------------------------|--|
| Ready biodegradability | - not readily biodegradable
(Manometric Respirometry Test, OECD No. 301 F) |
| Inherent biodegradability | - not inherently biodegradable
0 %, 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 as Dangerous Good according to the Dangerous Goods 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 17.05.1999) |
|------------------------------|--|

SECTION 16: Other information

- | | |
|-----------------------|---|
| Safety-lab number | - BS-5051 |
| 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.