

Chemical Safety Data Sheet MSDS / SDS

(3S,4aS,8aS)-N-tert-butyl-2-[(2R,3R)-2-hydroxy-3-[[3-hydroxy-2-(trideuteriomethyl)benzoyl]amino]-4-phenylsulfanylbutyl]-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinoline-3-carboxamide

Revision Date:2026-03-20 Revision Number:1

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

Product name : (3S,4aS,8aS)-N-tert-butyl-2-[(2R,3R)-2-hydroxy-3-[[3-hydroxy-2-(trideuteriomethyl)benzoyl]amino]-4-phenylsulfanylbutyl]-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinoline-3-carboxamide

CBnumber : CB73945224

CAS : 1217629-70-3

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.

Uses advised against : none

Company Identification

Company : Chemicalbook

Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing

Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS) : No data available

Signal word : No data available

Precautionary statements

No data available

Hazard statements

No data available

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

Product name : (3S,4aS,8aS)-N-tert-butyl-2-[(2R,3R)-2-hydroxy-3-[[3-hydroxy-2-(trideuteriomethyl)benzoyl]amino]-4-phenylsulfanylbutyl]-3,4,4a,5,6,7,8,8a-octahydro-1H-isoquinoline-3-carboxamide

CAS	: 1217629-70-3
MF	: C32H42D3N3O4S
MW	: 570.801

SECTION 4: First aid measures

Description of first aid measures

General information

No special measures required.

After inhalation

Supply fresh air; consult doctor in case of complaints.

After skin contact

Generally the product does not irritate the skin.

After eye contact

Rinse opened eye for several minutes under running water.

After swallowing

If symptoms persist consult doctor.

Most important symptoms and effects, both acute and delayed

No further relevant information available.

Indication of any immediate medical attention and special treatment needed

No further relevant information available.

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing agents

Use fire fighting measures that suit the environment.

A solid water stream may be inefficient.

Special hazards arising from the substance or mixture

No further relevant information available.

Advice for firefighters

Protective equipment

No special measures required.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Not required.

Environmental precautions

Do not allow to enter sewers/ surface or ground water.

Methods and material for containment and cleaning up

Pick up mechanically.

Protective Action Criteria for Chemicals

PAC-1

Substance is not listed.

PAC-2

Substance is not listed.

PAC-3

Substance is not listed.

Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

Precautions for safe handling

No special measures required.

Information about protection against explosions and fires

No special measures required.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Store in accordance with information listed on the product insert.

Storage

Store in accordance with information listed on the product insert.

Requirements to be met by storerooms and receptacles

No special requirements.

Information about storage in one common storage facility

Not required.

Further information about storage conditions

None.

Specific end use(s)

No further relevant information available.

SECTION 8: Exposure controls/personal protection

Control parameters

Components with limit values that require monitoring at the workplace

Not required.

Additional information

The lists that were valid during the creation were used as basis.

Exposure controls

Appropriate engineering controls

No further data; see section 7.

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Breathing equipment

Not required.

Protection of hands

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection

Not required.

SECTION 9: Physical and chemical properties**Information on basic physicochemical properties****Physical State**

Solid

Color

Not determined.

Odor

Characteristic

Structural Formula

C₃₂H₄₂D₃N₃O₄S

Molecular Weight

570.8 g/mol

Storage Buffer**Odor Threshold**

Not determined.

Formulation**Melting point/Melting range**

Undetermined.

Boiling point/Boiling range

Undetermined.

Flammability

Product is not flammable.

Explosion limits

Lower: Not determined.

Upper: Not determined.

Flash point

Not applicable.

Decomposition temperature

Not determined.

pH

Not applicable.

Viscosity**Kinematic**

Not applicable.

SOLUBILITY

DMSO: slightly soluble; Methanol: slightly soluble

Dynamic

Not applicable.

Solubility in / Miscibility with

DMSO: slightly soluble; Methanol: slightly soluble

Water

Not determined.

Partition coefficient (n-octanol/water)

Not determined.

Vapor Pressure

Not applicable.

Density

Not determined.

Relative Density

Not determined.

Vapor Density

Not applicable.

Particle characteristics

Not determined.

Other information**Appearance****Form**

Solid

Important information on protection of health and environment, and on safety.

Ignition temperature

Not determined.

Danger of explosion

Product does not present an explosion hazard.

Change in condition

Evaporation Rate

Not applicable.

SECTION 10: Stability and reactivity

Reactivity

No further relevant information available.

Chemical stability

Thermal decomposition / conditions to be avoided

No decomposition if used according to specifications.

Possibility of hazardous reactions

No dangerous reactions known.

Conditions to avoid

No further relevant information available.

Incompatible materials

strong oxidizing agents

Hazardous decomposition products

carbon oxides; nitrogen oxides; sulfur oxides

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

Primary irritant effect

on the skin

No irritant effect.

on the eye

No irritating effect.

Sensitization

No sensitizing effects known.

Additional toxicological information

When used and handled according to specifications, the product does not have any harmful effects according to our experience and the information provided to us.

The substance is not subject to classification.

Interactive effects

No interactive effects between components are known.

Carcinogenic categories**IARC (International Agency for Research on Cancer)**

Substance is not listed.

NTP (National Toxicology Program)

Substance is not listed.

OSHA-Ca (Occupational Safety & Health Administration)

Substance is not listed.

Alternative sources for toxicological information

No non-standard sources for toxicological information where used.

SECTION 12: Ecological information

Toxicity**Aquatic toxicity**

No further relevant information available.

Persistence and degradability

No further relevant information available.

Bioaccumulative potential

No further relevant information available.

Mobility in soil

No further relevant information available.

Results of PBT and vPvB assessment

PBT

Not applicable.

vPvB

Not applicable.

PBT:

Not applicable.

vPvB:

Not applicable.

Other adverse effects

Additional ecological information

General notes

Water hazard class 1 (Self-assessment) slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

SECTION 13: Disposal considerations

Waste treatment methods

Recommendation

Smaller quantities can be disposed of with household waste.

Uncleaned packagings

Recommendation

Disposal must be made according to official regulations.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA not regulated

UN proper shipping name

DOT, IMDG, IATA not regulated

Transport hazard class(es)

DOT, ADN, IMDG, IATA

Class not regulated

Packing group

DOT, IMDG, IATA not regulated

Environmental hazards

Not applicable.

Special precautions for user

Not applicable.

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

MARPOL73/78 and the IBC Code Not applicable.

UN "Model Regulation"

not regulated

SECTION 15: Regulatory information

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

No further relevant information available.

Sara

Section 355 (extremely hazardous substances):	Substance is not listed.
Section 313 (Specific toxic chemical listings):	Substance is not listed.
TSCA (Toxic Substances Control Act):	Substance is not listed.
Hazardous Air Pollutants:	Substance is not listed.
Chemicals known to cause cancer:	Substance is not listed.
Chemicals known to cause reproductive toxicity for females:	Substance is not listed.
Chemicals known to cause reproductive toxicity for males:	Substance is not listed.
Chemicals known to cause developmental toxicity:	Substance is not listed.

Carcinogenic categories

EPA (Environmental Protection Agency):	Substance is not listed.
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TLV (Threshold Limit Value)

Substance is not listed.

NIOSH-Ca (National Institute for Occupational Safety and Health)

Substance is not listed.

Chemical safety assessment

SECTION 16: Other information

Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.