

Chemical Safety Data Sheet MSDS / SDS

N-[(1R,2R)-1,2-Diphenyl-2-(2-(4-Methylbenzyloxy)ethyl)amino)-ethyl]-4-Methylbenzene sulfonamide(chloro)ruthenium(II) (R,R)-Ts-DENEb 1333981-84-2

Revision Date:2026-05-31 Revision Number:1

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

Product name : N-[(1R,2R)-1,2-Diphenyl-2-(2-(4-Methylbenzyloxy)ethyl)amino)-ethyl]-4-Methylbenzene sulfonamide(chloro)ruthenium(II) (R,R)-Ts-DENEb 1333981-84-2

CBnumber : CB42709408

CAS : 1333981-84-2

Synonyms : (R,R)-Ts-DENEb, N-[(1R,2R)-1,2-Diphenyl-2-(2-(4-Methylbenzyloxy)ethyl)amino)-ethyl]-4-Methylbenzene sulfonamide(chloro)ruthenium(II)

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)



Signal word

Warning

Precautionary statements

P405 Store locked up.

P308+P313 IF exposed or concerned: Get medical advice/attention.

P391 Collect spillage. Hazardous to the aquatic environment

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P201 Obtain special instructions before use.

P202 Do not handle until all safety precautions have been read and understood.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P273 Avoid release to the environment.

P501 Dispose of contents/container to.....

Hazard statements

H411 Toxic to aquatic life with long lasting effects

H351 Suspected of causing cancer

H373 May cause damage to organs through prolonged or repeated exposure

SECTION 3: Composition/information on ingredients

Substance

Product name	: N-[(1R,2R)-1,2-Diphenyl-2-(2-(4-Methylbenzyloxy)ethylamino)-ethyl]-4-Methylbenzene sulfonamide(chloro)ruthenium(II) (R,R)-Ts-DENEb 1333981-84-2
Synonyms	: (R,R)-Ts-DENEb,N-[(1R,2R)-1,2-Diphenyl-2-(2-(4-Methylbenzyloxy)ethylamino)-ethyl]-4-Methylbenzene sulfonamide(chloro)ruthenium(II)
CAS	: 1333981-84-2
MF	: C ₃₁ H ₃₃ ClN ₂ O ₃ RuS
MW	: 650.2

SECTION 4: First aid measures

If inhaled

Remove person to fresh air and keep comfortable for breathing. Get medical advice/ attention.

In case of skin contact

Take off all contaminated clothing immediately. If on skin, rinse well with water. Get medical advice/ attention.

In case of eye contact

Rinse with plenty of water. If easy to do, remove contact lens, if worn. Get medical advice/ attention.

If swallowed

Get medical advice/ attention. Rinse mouth.

Most important symptoms and effects, both acute and delayed

None known.

SECTION 5: Firefighting measures

Suitable extinguishing media

Dry powder, Foam, Water spray, Carbon dioxide (CO₂)

Specific hazards during fire fighting

No information available.

Specific extinguishing methods

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Immediately evacuate personnel to safe areas. Remove undamaged containers from fire area if it is safe to do so.

Special protective equipment for fire-fighters

Use personal protective equipment.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear suitable protective equipment. Keep people away from and upwind of spill/leak. Entry to non-involved personnel should be controlled around the leakage area by roping off, etc.

Environmental precautions

Should not be released into the environment.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust.

SECTION 7: Handling and storage

Handling

Technical measures

Prevent dispersion of dust.

Local/Total ventilation

Ensure adequate ventilation. Handle product only in closed system or provide appropriate exhaust ventilation at machinery. Use a local exhaust ventilation.

Advice on safe handling

Avoid contact with skin, eyes and clothing. Wear personal protective equipment. Wash hands and face thoroughly after handling.

Avoidance of contact

Oxidizing agents

Storage

Conditions for safe storage

Keep container tightly closed. Store in a cool and shaded area. Keep under inert gas. Store locked up.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Components	CAS RN	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
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4-Methyl-2-pentanone	108-10-1	TWA	20 ppm	ACGIH
		STEL	75 ppm	ACGIH
Heptane	142-82-5	PC-TWA	500 mg/m3	CN OEL
		PC-STEL	1,000 mg/m3	CN OEL
		TWA	400 ppm	ACGIH
		STEL	500 ppm	ACGIH

Components CAS RN Value type Control parameters Basis (Form of ex- / Permissible conposure) centration 4-Methyl-2-pentanone 108-10-1

TWA 20 ppm ACGIH

STEL 75 ppm ACGIH

Heptane 142-82-5 PC-TWA 500 mg/m3 CN OEL

PC-STEL 1,000 mg/m3 CN OEL

TWA 400 ppm ACGIH

STEL 500 ppm ACGIH

Engineering measures

Install a closed system or local exhaust.

Also install safety shower and eye bath.

Personal protective equipment

Respiratory protection

Dustproof gas mask

Self-contained breathing apparatus

Eye/face protection

Safety glasses

Safety goggles

Face-shield

Skin and body protection

Impervious protective clothing

Hand protection

Impervious gloves *Use personal protective equipment(PPE) approved under appropriate government standards and follow local and national regulations.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

solid

Color

white - yellow

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/freezing point

No data available

Boiling point/boiling range

No data available

Flash point

No data available

Evaporation rate

No data available

Flammability

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Solubility(ies)**Water solubility**

No data available

Solubility in other solvents

No data available

Partition coefficient: n-octanol/water (log value)

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Molecular weight

650.20 g/mol

Physical state

solid

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under normal conditions.

Possibility of hazardous reactions

None under normal processing.

Conditions to avoid

Exposure to air.

Incompatible materials

Oxidizing agents

Hazardous decomposition products

Carbon monoxide, Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Hydrogen chloride gas, Metal oxides

SECTION 11: Toxicological information

Acute toxicity

Product

Acute oral toxicity

Acute toxicity estimate: > 5,000 mg/kg Method: Calculation method

Acute inhalation toxicity

Acute toxicity estimate: > 10 mg/l Exposure time: 4 h Test atmosphere: dust/mist Method: Calculation method

Acute dermal toxicity

Acute toxicity estimate: > 5,000 mg/kg Method: Calculation method

Components

3-Methoxy-1-propanol

Acute oral toxicity

LD50 (Rat): 5,710 mg/kg Assessment: The substance or mixture has no acute oral toxicity

Acute dermal toxicity

LD50 (Rabbit): 5,320.4 mg/kg Assessment: The substance or mixture has no acute dermal toxicity

4-Methyl-2-pentanone

Acute oral toxicity

LD50 (Rat): 2,080 mg/kg Assessment: The component/mixture is minimally toxic after single ingestion.

Acute inhalation toxicity

Assessment: The component/mixture is moderately toxic after short term inhalation.

Acute toxicity (other routes of administration)

LD50 (Rat): 400 mg/kg Application Route: Intraperitoneal injection

Heptane

Acute inhalation toxicity

TCLo (Humans): 1000 ppm Exposure time: 6 min Test atmosphere: gas Assessment: The substance or mixture has no acute inhalation toxicity

LC50 (Rat)

103 g/m³ Exposure time: 4 h Test atmosphere: dust/mist

Acute dermal toxicity

Assessment: The component/mixture is minimally toxic after single contact with skin.

Acute toxicity (other routes of administration)

LD50 (Mouse): 222 mg/kg Application Route: Intravenous

Skin corrosion/irritation

Components

Heptane

Result

Skin irritation

Serious eye damage/eye irritation

Components

4-Methyl-2-pentanone

Result

Eye irritation

Heptane

Result

Mild eye irritation

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2.

Germ cell mutagenicity

Classified based on available data. For more details, see section 2.

Carcinogenicity

Components

4-Methyl-2-pentanone

Carcinogenicity - Assessment

Suspected human carcinogens

Reproductive toxicity

Classified based on available data. For more details, see section 2.

STOT-single exposure

Components

4-Methyl-2-pentanone

Assessment

May cause respiratory irritation. May cause drowsiness or dizziness.

Heptane

Assessment

May cause respiratory irritation. May cause drowsiness or dizziness.

STOT-repeated exposure

Product

Target Organs

Nervous system

Assessment

May cause damage to organs through prolonged or repeated exposure.

Components

4-Methyl-2-pentanone

Target Organs

Nervous system

Assessment

Causes damage to organs through prolonged or repeated exposure.

Repeated dose toxicity

Classified based on available data. For more details, see section 2.

Aspiration toxicity

Components

Heptane

RTECS No.

UB7650000 (3-Methoxy-1-propanol) SA9275000 (4-Methyl-2-pentanone) MI7700000 (Heptane)

SECTION 12: Ecological information

Ecotoxicity

Components: (R,R)-Ts-DENEBO®:

Ecotoxicology Assessment

Acute aquatic toxicity

Harmful to aquatic life.

Chronic aquatic toxicity

Harmful to aquatic life with long lasting effects.

Heptane:

Ecotoxicology Assessment

Acute aquatic toxicity

Very toxic to aquatic life.

Chronic aquatic toxicity

Very toxic to aquatic life with long lasting effects.

Persistence and degradability

No data available

Bioaccumulative potential

Components:

4-Methyl-2-pentanone:

octanol/water (log value)

Partition coefficient: octanol/water (log value)

1.38

Heptane:

octanol/water (log value)

Partition coefficient: octanol/water (log value)

4.66

Mobility in soil

Components:

4-Methyl-2-pentanone:

tal compartments

Distribution among environmental compartments

Koc: 123

Heptane:

tal compartments

Distribution among environmental compartments

Koc: 240

Other adverse effects

No data available

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Disposal in accordance with local and national regulations. Entrust disposal to a licensed waste disposal company.

Contaminated packaging

Disposal in accordance with local and national regulations. Before disposal of used container, remove contents completely.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No.

Not applicable

Proper shipping name

Not applicable

Class

Not applicable

Subsidiary risk

Not applicable

Packing group

Not applicable

IMDG-Code

UN number

Not applicable

Proper shipping name

Not applicable

Class

Not applicable

Subsidiary risk

Not applicable

Packing group

Not applicable

EmS Code

Not applicable

Domestic regulation

GB 6944/12268

UN number

Not applicable

Proper shipping name

Not applicable

Class

Not applicable

Subsidiary risk

Not applicable

Packing group

Not applicable

SECTION 15: Regulatory information

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A232216155

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

The ingredients of this product are reported in the following inventories

TCSI

Not in compliance with the inventory

TSCA

Product contains substance(s) not listed on TSCA inventory.

AIRC

Not in compliance with the inventory

DSL

This product contains the following components that are not on the Canadian DSL nor NDSL.

(R,R)-Ts-DENEBO®

ENCS

Not in compliance with the inventory

ISHL

Not in compliance with the inventory

KECI

Not in compliance with the inventory

PICCS

Not in compliance with the inventory

IECSC

Not in compliance with the inventory

NZIOB

Not in compliance with the inventory

TECI

Not in compliance with the inventory

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.