ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

ACETIC ACID (2R,3R,4R,5R)-3,4-DIACETOXY-5-(6-CHLORO-2-IODO-PURIN-9-YL)-TETRAHYDRO-FURAN-2-YLMETHYL ESTER

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

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

Product identifier

Product name	: ACETIC ACID (2R,3R,4R,5R)-3,4-DIACETOXY-5-(6-CHLORO-2-IODO-PURIN-9-YL)-TETRAHYDRO-FURAN-2-YLMETHYL ESTER
CBnumber	: CB51011040
CAS	: 5987-76-8
Synonyms	: (2R,3R,4R,5R)-2-(acetoxymethyl)-5-(6-chloro-2-iodo-9H-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate

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

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

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

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

Hazard statements

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: ACETIC ACID (2R,3R,4R,5R)-3,4-DIACETOXY-5-(6-CHLORO-2-IODO-PURIN-9-YL)-TETRAHYDRO-FURAN-2-YLMETHYL ESTER
Synonyms	: (2R,3R,4R,5R)-2-(acetoxymethyl)-5-(6-chloro-2-iodo-9H-purin-9-yl)tetrahydrofuran-3,4-diyl diacetate
CAS	: 5987-76-8
MF	: C16H16ClIN4O7
MW	: 538.68

SECTION 4: First aid measures

If inhaled

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

In case of skin contact

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

In case of eye contact

Rinse with plenty of water. If easy to do, remove contact lens, if worn. If eye irritation persists: 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

Prevent product from entering drains.

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. 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.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

Install a closed system or local exhaust.

Also install safety shower and eye bath.

Personal protective equipment

Respiratory protection

Dust mask

Eye/face protection

Safety glasses

Face-shield

Skin and body protection

Protective suit

Hand protection

Protective 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

184 °C

Boiling point/boiling range

643.3±65.0 °C(Predicted)

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)

Dichloromethane, Ether, Ethyl Acetate, Methanol

Water solubility

No data available

Solubility in other solvents

Dichloromethane, Ether, Ethyl Acetate, Methanol

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

538.68 g/mol

Density and/or relative density

1.98±0.1 g/cm3(Predicted)

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.

Incompatible materials

Oxidizing agents

Hazardous decomposition products

Carbon monoxide, Carbon dioxide (CO2), Nitrogen oxides (NOx), Hydrogen chloride gas, Hydrogen halides

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SECTION 11: Toxicological information

Acute toxicity

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

Skin corrosion/irritation

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

Serious eye damage/eye irritation

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

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

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

Reproductive toxicity

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

STOT-single exposure

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

STOT-repeated exposure

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

Repeated dose toxicity

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

Aspiration toxicity

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

SECTION 12: Ecological information

Ecotoxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

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

B1A232233765

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

CH BAGREG

Not in compliance with the inventory

TSCA

Substance(s) not listed on TSCA inventory

AICS

Not in compliance with the inventory

DSL

This product contains the following components that are not on the

Canadian DSL nor NDSL.

2',3',5'-Tri-O-acetyl-6-chloro-2-iodopurine Riboside

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

NZIoC

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