

## Chemical Safety Data Sheet MSDS / SDS

**BENZOIC ACID, 2-[[[(1,1-DIMETHYLETHOXY)CARBONYL]AMINO]-3-NITRO-METHYL ESTER**Revision Date:2026-05-16 Revision Number:1

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

Product name : BENZOIC ACID, 2-[[[(1,1-DIMETHYLETHOXY)CARBONYL]AMINO]-3-NITRO-METHYL ESTER  
CBnumber : CB2784463  
CAS : 57113-90-3  
EINECS Number : 611-470-7  
Synonyms : 2-(tert-butoxycarbonylamino)-3-nitrobenzoic acid methyl ester,BENZOIC ACID, 2-[[[(1,1-DIMETHYLETHOXY)CARBONYL]AMINO]-3-NITRO-METHYL ESTER

**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

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**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

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

Product name : BENZOIC ACID, 2-[[[(1,1-DIMETHYLETHOXY)CARBONYL]AMINO]-3-NITRO-METHYL ESTER

Synonyms	: 2-(tert-butoxycarbonylamino)-3-nitrobenzoic acid methyl ester,BENZOIC ACID, 2-[[[1,1-DIMETHYLETHOXY)CARBONYL]AMINO]-3-NITRO-METHYL ESTER
CAS	: 57113-90-3
EC number	: 611-470-7
MF	: C13H16N2O6
MW	: 296.28

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## 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.

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## SECTION 5: Firefighting measures

### **Suitable extinguishing media**

Dry powder, Foam, Water spray, Carbon dioxide (CO<sub>2</sub>)

### **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.

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## 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.

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## **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.

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## **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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

solid

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#### Color

white - yellow

#### Odor

No data available

#### Odor Threshold

No data available

#### pH

No data available

#### Melting point/freezing point

106 °C

#### Boiling point/boiling range

376.9±32.0 °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

**Water solubility**

No data available

**Solubility in other solvents**

Dichloromethane

**Partition coefficient: n-octanol/water**

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**

296.28 g/mol

**Density and/or relative density**

1.298±0.06 g/cm<sup>3</sup>(Predicted)

**Physical state**

Solid

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## 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 (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>)

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## SECTION 11: Toxicological information

### **Acute toxicity**

No information available.

### **Skin corrosion/irritation**

No information available.

### **Serious eye damage/eye irritation**

No information available.

### **Respiratory or skin sensitization**

No information available.

### **Germ cell mutagenicity**

No information available.

### **Carcinogenicity**

No information available.

### **Reproductive toxicity**

No information available.

### **STOT-single exposure**

No information available.

### **STOT-repeated exposure**

No information available.

### **Repeated dose toxicity**

No information available.

### **Aspiration toxicity**

No information available.

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## 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

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## 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.

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## 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

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## SECTION 15: Regulatory information

**Measures on the Environmental Administration of New Chemical Substances Registration****Registration/Notification number**

B1A232215092

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.

Methyl 2-(tert-Butoxycarbonylamino)-3-nitrobenzoate

**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

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## 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.