

Chemical Safety Data Sheet MSDS / SDS

tert-butyl 4-(2-amino-4-bromophenyl)piperazine-1-carboxylateRevision Date:2026-05-31 Revision Number:1

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

Product name : tert-butyl 4-(2-amino-4-bromophenyl)piperazine-1-carboxylate
CBnumber : CB61561764
CAS : 474329-58-3
Synonyms : 1-Piperazinecarboxylic acid, 4-(2-amino-4-bromophenyl)-, 1,1-dimethylethyl 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

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

Symbol(GHS)



Signal word

Warning

Precautionary statements

P337+P313 IF eye irritation persists: Get medical advice/attention.
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P264 Wash skin thoroughly after handling.

Hazard statements

H319 Causes serious eye irritation
H315 Causes skin irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: tert-butyl 4-(2-amino-4-bromophenyl)piperazine-1-carboxylate
Synonyms	: 1-Piperazinecarboxylic acid, 4-(2-amino-4-bromophenyl)-, 1,1-dimethylethyl ester
CAS	: 474329-58-3
MF	: C ₁₅ H ₂₂ BrN ₃ O ₂
MW	: 356.26

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen bromide gas

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact.

Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

Storage class

Storage class (TRGS 510): 11: Combustible Solids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 L

Body Protection

protective clothing

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	solid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	465.1±45.0 °C(Predicted)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive	No data available

limits	
h) Flash point	Not applicable
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	at 25 °C slightly soluble
n) Partition coefficient n-octanol/water	log Pow: 4.39 at 25 °C - Potential bioaccumulation
o) Vapor pressure	No data available
p) Density	1.378±0.06 g/cm ³ (Predicted)
Relative density	1.378±0.06 g/cm ³ (Predicted)
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

no information available

10.4 Incompatible materials

Strong oxidizing agents

10.5 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 1,790 mg/kg (Expert judgment)

Remarks: The value / statement given is based on a (Q)SAR approach

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: The value / statement given is based on a (Q)SAR approach

Serious eye damage/eye irritation

Remarks: The value / statement given is based on a (Q)SAR approach

Respiratory or skin sensitization

The value / statement given is based on a (Q)SAR approach

Germ cell mutagenicity

Test Type: Ames test

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

Test Type: Chromosome aberration test in vitro

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

Test Type: Micronucleus test

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

Test Type: comet assay

Method: QSAR

Result: positive

Remarks: The value / statement given is based on a (Q)SAR approach

Carcinogenicity

Potential cancer hazard.

Reproductive toxicity

see user defined free text

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

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

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

Biodegradability

Result: - Not readily biodegradable.

Remarks: The value / statement given is based on a (Q)SAR approach

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 3077

IMDG: 3077

IATA-DGR: 3077

14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (tert-butyl 4- (2-amino-4-bromophenyl)-1-piperazinecarboxylate)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (tert-butyl 4- (2-amino-4-bromophenyl)-1-piperazinecarboxylate)

IATA-DGR: Environmentally hazardous substance, solid, n.o.s. (tert-butyl 4-(2-amino-4- bromophenyl)-1-piperazinecarboxylate)

14.3 Transport hazard class(es)

ADR/RID: 9

IMDG: 9

IATA-DGR: 9

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA-DGR: III

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA-DGR: yes

14.6 Special precautions for user

14.7 Incompatible materials

Strong oxidizing agents

Further information: EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of

Class 9

SECTION 15: Regulatory information

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

National regulatory information

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222223214

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.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

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.