

1. Identification

1.1 GHS Product identifier

Product name tert-butyl 2-methylsulfonyl-5,7-dihydropyrrolo[3,4-d]pyrimidine-6-carboxylate

1.2 Other means of identification

Product number PYR629

Other names N/A

1.3 Recommended use of the chemical and restrictions on use

Identified uses For industry use only.

Uses advised against no data available

1.4 Supplier's details

Company Acros PharmaTech Limited

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2. Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s) no data available
Signal word no data available
Hazard statement(s) no data available
Precautionary statement(s)
Prevention no data available
Response no data available
Storage no data available
Disposal no data available

2.3 Other hazards which do not result in classification

no data available

3. Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
tert-butyl	tert-butyl			
2-methylsulfonyl-5,7-dihydropyrrolo[3,4-d]pyrimidine-6-carboxylate	2-methylsulfonyl-5,7-dihydropyrrolo[3,4-d]pyrimidine-6-carboxylate	365996-87-8	none	≥97%

4. First-aid measures

4.1 Description of necessary first-aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms/effects, acute and delayed

no data available

4.3 Indication of immediate medical attention and special treatment needed, if necessary

no data available

5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Specific hazards arising from the chemical

no data available

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal. Sweep up and shovel. Keep in suitable, closed containers for disposal.

7. Handling and storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Avoid exposure - obtain special instructions before use. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

8. Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Safety glasses with side-shields conforming to EN166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Wear impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace. Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

Wear dust mask when handling large quantities.

Thermal hazards

no data available

9. Physical and chemical properties

Physical state	no data available
Colour	no data available
Odour	no data available
Melting point/ freezing point	no data available
Boiling point or initial boiling point and boiling range	481.207°C at 760 mmHg
Flammability	no data available

Lower and upper explosion limit / flammability limit	no data available
Flash point	244.825°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water (log value)	no data available
Vapour pressure	no data available
Density and/or relative density	1.33g/cm ³
Relative vapour density	no data available
Particle characteristics	no data available

10. Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

11. Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

12. Ecological information**12.1 Toxicity**

- Toxicity to fish: no data available
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Other adverse effects

no data available

13. Disposal considerations**13.1 Disposal methods****Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be

punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

14. Transport information

14.1 UN Number

ADR/RID: no data available IMDG: no data available IATA: no data available

14.2 UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

14.3 Transport hazard class(es)

ADR/RID: no data available IMDG: no data available IATA: no data available

14.4 Packing group, if applicable

ADR/RID: no data available IMDG: no data available IATA: no data available

14.5 Environmental hazards

ADR/RID: no IMDG: no IATA: no

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

no data available

15. Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
tert-butyl	tert-butyl	365996-87-8	none
2-methylsulfonyl-5,7-dihydropyrrolo[3,4-d]pyrimidine-6-carboxylate	2-methylsulfonyl-5,7-dihydropyrrolo[3,4-d]pyrimidine-6-carboxylate		
European Inventory of Existing Commercial Chemical Substances (EINECS)			Not Listed.
EC Inventory			Not Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Not Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
New Zealand Inventory of Chemicals (NZIoC)			Not Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Not Listed.
Vietnam National Chemical Inventory			Not Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Not Listed.

16. Other information

Abbreviations and acronyms

- CAS: Chemical Abstracts Service

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- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
 - RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
 - IMDG: International Maritime Dangerous Goods
 - IATA: International Air Transportation Association
 - TWA: Time Weighted Average
 - STEL: Short term exposure limit
 - LC50: Lethal Concentration 50%
 - LD50: Lethal Dose 50%
 - EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product.