

SAFETY DATA SHEET

Version 6.3
Revision Date 10/08/2021
Print Date 06/02/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Pyrasulfotole

Product Number : 32973
Brand : Sigma-Aldrich
CAS-No. : 365400-11-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram none

Signal word none

Hazard statement(s)
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)
P273 Avoid release to the environment.
P501 Dispose of contents/ container to an approved waste disposal

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plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-p-tolyl)methanone
(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone

Formula : $C_{14}H_{13}F_3N_2O_4S$

Molecular weight : 362.32 g/mol

CAS-No. : 365400-11-9

No components need to be disclosed according to the applicable regulations.

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material 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 and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Nitrogen oxides (NO_x)
Sulfur oxides
Hydrogen fluoride
Nature of decomposition products not known.
Carbon oxides
Nitrogen oxides (NO_x)
Sulfur oxides
Hydrogen fluoride

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. 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 without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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

Keep in a dry place.

Storage class

Storage class (TRGS 510): 13: Non Combustible Solids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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**

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

Personal protective equipment**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

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.

Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

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

SECTION 9: Physical and chemical properties**9.1 Information on basic physical and chemical properties**

- | | |
|-------------------|-------------------------------------|
| a) Appearance | Form: powder
Color: beige |
| b) Odor | odorless |
| c) Odor Threshold | No data available |
| d) pH | ca.3 at 10 g/l at 22.9 °C (73.2 °F) |
| e) Melting | 201 °C (394 °F) |

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	point/freezing point	
f)	Initial boiling point and boiling range	No data available
g)	Flash point	()No data available
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	1.5 g/cm ³ at 20 °C (68 °F)
	Relative density	No data available
n)	Water solubility	69 g/l at 20 °C (68 °F)
o)	Partition coefficient: n-octanol/water	log Pow: -1.362 at 23 °C (73 °F)
p)	Autoignition temperature	No data available
q)	Decomposition temperature	> 245 °C (> 473 °F), 3 K/min -
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Solubility in other solvents	Acetone 89.2 g/l at 20 °C (68 °F)
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SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Dust can form an explosive mixture in air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents, Strong reducing agents

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10.6 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 - 2,500 mg/kg

(Calculation method)

LD50 Oral - Rat - > 2,000 mg/kg

Acute toxicity estimate Inhalation - 5.25 mg/l

(Calculation method)

LC50 Inhalation - Rat - 4 h - > 5.030 mg/l

Acute toxicity estimate Dermal - 2,500 mg/kg

(Calculation method)

LD50 Dermal - Rat - > 2,000 mg/kg

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Mild eye irritation

Respiratory or skin sensitization

- Guinea pig

Did not cause sensitization on laboratory animals.

(OECD Test Guideline 406)

Germ cell mutagenicity

In vivo tests did not show mutagenic effects Tests on bacterial or mammalian cell cultures did not show mutagenic effects.

Carcinogenicity

The observed tumors do not appear to be relevant for men.

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

Animal testing did not show any effects on fetal development.

No toxicity to reproduction

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - Oral - NOAEL (No observed adverse effect level) - > 500 mg/kg

Repeated dose toxicity - Mouse - Oral - NOAEL (No observed adverse effect level) - > 500 mg/kg

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	LC50 - <i>Lepomis macrochirus</i> (Bluegill) - > 100 mg/l - 96.0 h
	LC50 - <i>Oncorhynchus mykiss</i> (rainbow trout) - > 100 mg/l - 96.0 h
	LC50 - <i>Cyprinodon variegatus</i> (sheepshead minnow) - > 100 mg/l - 96.0 h
Toxicity to daphnia and other aquatic invertebrates	EC50 - <i>Daphnia magna</i> (Water flea) - > 100 mg/l - 48 h
Toxicity to algae	EC50 - <i>Pseudokirchneriella subcapitata</i> - 29.8 mg/l - 96 h

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
(Directive 67/548/EEC Annex V, C.4.D.)

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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life.

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

No SARA Hazards

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

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New Jersey Right To Know Components

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California Prop. 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

SECTION 16: Other information

Further information

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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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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