

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Riluzole Related Compound A, United States Pharmacopeia (USP) Reference Standard

Product Number : 1604348
Brand : US Pharmacopeia
CAS-No. : 461-82-5

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : Not Available

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
SPRUCE ST 3050
63103 St. Louis

Telephone : (314) 771-5765
Telefax: (800) 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800 424 9300 (CHEMTREC) 24/7
+1 703 527 3887 (CHEMTREC) 24/7

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 4



Acute toxicity (Oral) : Category 3

Acute toxicity (Dermal) : Category 2

Skin irritation : Category 2

Serious eye damage : Category 1

Specific target organ toxicity - repeated exposure : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H227 Combustible liquid.
H301 Toxic if swallowed.
H310 Fatal in contact with skin.
H315 Causes skin irritation.
H318 Causes serious eye damage.
H373 May cause damage to organs through prolonged or repeated exposure.

Precautionary statements : **Prevention:**
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P262 Do not get in eyes, on skin, or on clothing.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/ eye protection/ face protection.

Response:
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P350 + P310 IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.
P302 + P352 IF ON SKIN: Wash with plenty of soap and



water.

P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P314 Get medical advice/ attention if you feel unwell.

P332 + P313 If skin irritation occurs: Get medical advice/ attention.

P362 Take off contaminated clothing and wash before reuse.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

P403 + P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 461-82-5

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
4-(Trifluoromethoxy)aniline	461-82-5*	$\geq 90 - \leq 100$	-

* Indicates that the identifier is a CAS No.

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Call in physician.

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

In case of eye contact : After eye contact: rinse out with plenty of water.

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Immediately call in ophthalmologist.
Remove contact lenses.

If swallowed	: If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.
Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Vapours are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating.
Hazardous combustion products	: Carbon oxides Nitrogen oxides (NO _x) Hydrogen fluoride
Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.



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

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapours, aerosols.
Avoid substance contact.
Ensure adequate ventilation.
Keep away from heat and sources of ignition.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
Wear appropriate personal protective equipment, as indicated in Section 8.

Environmental precautions : Do not let product enter drains.

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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.

Further information on storage conditions : Tightly closed.
Keep in a well-ventilated place.
Keep locked up or in an area accessible only to qualified or authorised persons.



Storage class : 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols 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.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Tightly fitting safety goggles

Skin and body protection : protective clothing

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



SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid
Colour	: yellow
Odour	: No data available
Odour Threshold	: No data available
pH	: No data available
Melting point	: No data available
Boiling point/boiling range	: 163 - 167 °F / 73 - 75 °C (13 hPa)
Flash point	: 178 °F / 81 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapour pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.320 g/cm ³
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available



Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Molecular weight	: 177.13 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Strong heating.
Incompatible materials	: Strong oxidizing agents
Hazardous decomposition products	: For Hazardous combustion products in the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 132 mg/kg

Inhalation: No data available

LD50 Dermal - Rat - 105 mg/kg

No data available

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada



Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Severe eye irritation

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Result: Not mutagenic in Ames Test

Remarks: Histidine reversion (Ames)

Carcinogenicity

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

NTP: No component 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

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

No data available

11.2 Additional Information

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12. ECOLOGICAL INFORMATION**Ecotoxicity****Components:****4-(Trifluoromethoxy)aniline:**

Toxicity to fish : Remarks: No data available



Persistence and degradability

Components:

4-(Trifluoromethoxy)aniline:

Biodegradability : Remarks: No data available

Bioaccumulative potential

Components:

4-(Trifluoromethoxy)aniline:

Bioaccumulation : Remarks: No data available

Mobility in soil

Components:

4-(Trifluoromethoxy)aniline:

Stability in soil : Remarks: No data available

Other adverse effects

Components:

4-(Trifluoromethoxy)aniline:

Additional ecological information : No data available

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 2941
Proper shipping name : Fluoroanilines
Class : 6.1
Packing group : III
Labels : Division 6.1 - Toxic substances

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Packing instruction (cargo : 663
aircraft)
Packing instruction : 655
(passenger aircraft)

IMDG-Code

UN number : UN 2941
Proper shipping name : FLUOROANILINES

Class : 6.1
Packing group : III
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 2941
Proper shipping name : Fluoroanilines

Class : 6.1

Packing group : III
Labels : Division 6.1 - Toxic substances
ERG Code : 153
Marine pollutant : no
Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
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SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard



SARA 313 : 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.

US State Regulations

Massachusetts Right To Know

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

Pennsylvania Right To Know

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Pennsylvania Right To Know

4-(Trifluoromethoxy)aniline 461-82-5

New Jersey Right To Know

4-(Trifluoromethoxy)aniline 461-82-5

California Prop. 65

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

The components of this product are reported in the following inventories:

US TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing

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Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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