1. Identification of the substance/mixture and of the company/undertaking

1.1. Product Details

Product Code : M491
Name : Tris(2-(benzo[b]thiophen-2-yl)pyridineiridium(III)
REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration or the annual tonnage does not require a registration.
CAS No. : 405289-74-9

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

Identified uses : Laboratory chemicals

1.3. Supplier details

Supplied by : Ossila Limited
Kroto Innovation Centre
Broad Lane, Sheffield
S3 7HQ, UK
Telephone : 0114 213 2770
Email address : info@ossila.com

2. Hazards identification

2.1. Classification of the substance or mixture

Hazard statements according to Regulation (EC) 1272/2008
Skin irritation (Category 2), H315
Eye irritation (Category 2), H319
Specific target organ toxicity - single exposure (Category 3), H335

2.2. Label elements

Labelling according Regulation (EC) No 1272/2008 [CLP]

Signal word
Warning

Hazard statement(s)
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation

Precautionary statement(s)
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental information
None.
2.3. Other hazards
None.

3. Composition/Information on ingredients

3.1. Substances
Synonyms: \( \text{Ir(btpy)}_3, \text{Tris}[2\{-\text{benzo}[b]\text{thiophen}-2\text{-yl}\}\text{pyridinato-C3,N}]\text{iridium(III)}, \)
\( \text{fac-Tris}[2\{-\text{benzo}[b]\text{thiophen}-2\text{-yl}\}\text{pyridinato-C3,N}]\text{iridium(III)}, \)
\( \text{fac-Ir(btpy)}_3, \text{Tris}[2\{-\text{benzo}[b]\text{thiophen}-2\text{-yl}\}\text{pyridineiridium(III)} \)
Formula: \( \text{C}_{39}\text{H}_{24}\text{IrN}_3\text{S}_3 \)
Molecular weight: 823.08 g/mol

Hazardous ingredients according to Regulation (EC) No 1272/2008

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS #</th>
<th>Weight %</th>
<th>CLP Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tris[2{-\text{benzo}[b]\text{thiophen}-2\text{-yl}}\text{pyridineiridium(III)}</td>
<td>405289-74-9</td>
<td>≤ 100</td>
<td>Skin irrit. 2 (H315), Eye irrit. 2 (H319), STOT SE 3 (H335)</td>
</tr>
</tbody>
</table>

4. First aid measures

4.1. Description of first aid measures
After Inhalation
If inhaled, remove to fresh air. If not breathing give artificial respiration. Call a physician.

After skin contact
In case of skin contact, wash with soap and flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

After eye contact
In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

After Ingestion
If swallowed, wash out mouth with water. Call a physician.

4.2. Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in section 11.

4.3. Indication of any immediate medical attention and special treatment needed
No data available.

5. Fire fighting

5.1. Extinguishing media
Suitable extinguishing media: Dry chemical, alcohol-resistant foam, carbon dioxide or water spray. Consult with local fire authorities before attempting large scale fire fighting operations.

5.2. Special hazards arising from the substance of mixture
Hazardous combustion products: Carbon oxides, nitrogen oxides, sulfur oxides, iridium oxides.

5.3. Advice for firefighters
Wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. During a fire, irritating and highly toxic gases and vapours may be generated by thermal decomposition.
6. Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures
Wear personal protective equipment (section 8). Avoid dust formation. Ensure room is well ventilated. Remove all sources of ignition.

6.2. Environmental precautions
Do not let product enter drains.

6.3. Containment and cleaning
Contain and clean up spill if safe to do so using an electrically protected vacuum cleaner or by wet-brushing. Dispose of dry waste in closed container for proper disposal according to local regulations.

7. Handling and storage

7.1. Precautions for safe handling
Avoid formation of dust and aerosols. Keep away from sources of ignition and avoid the build up of electrostatic charge. Provide exhaust ventilation in places where dust is formed.

7.2. Conditions for safe storage, including any incompatibilities
Store in a cool, dry and well-ventilated place inside of a tightly sealed container. Reseal containers that have been opened and keep upright to prevent leakage.

7.3. Specific end uses
Use in laboratories.

8. Exposure controls / Personal protection

8.1. Control parameters
Components with workplace control parameters
Contains no substances with occupational exposure limit values.

Biological occupational exposure limits
This product does not contain any hazardous materials with biological limits.

8.2. Exposure controls
Engineering measures
Handle in accordance with good industrial engineering/laboratory practices for hygiene and safety. Ensure eyewash stations and safety showers are close to the laboratory workstation. Ensure good general ventilation is present when handling the product.

Personal protective equipment
Eyes: Wear safety glasses with side-shields conforming to appropriate government standards such as NOISH (US) or EN166 (EU).
Skin: Handle with appropriate gloves and use proper glove removal technique to avoid skin contact. Dispose of gloves in accordance with applicable laws. 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.
Clothing: Wear complete suit protecting against chemicals; the type of equipment should be appropriate for the concentration and amount of dangerous substance used.
Respirators: A respiratory protection program that meets OSHA’s 29 CFR §1910.134 and ANSI Z88.2 requirements or European standard EN 149 must be followed whenever workplace conditions warrant a respirator’s use.

General hygiene measures
Wash thoroughly after handling. Wash contaminated clothing before reuse.

9. Physical and chemical properties

9.1. Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Solid red powder</td>
</tr>
<tr>
<td>Odour</td>
<td>No data available</td>
</tr>
<tr>
<td>Odour threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>&gt; 300 °C</td>
</tr>
<tr>
<td>Boiling point/range</td>
<td>No data available</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapour density</td>
<td>No data available</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Solubility(ies)</td>
<td>No data available</td>
</tr>
<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>No data available</td>
</tr>
<tr>
<td>Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2. Other safety information
No data available.

10. Stability and reactivity

10.1 Reactivity
No data available.

10.2. Chemical stability
Stable under normal temperatures and pressures under recommended storage conditions.

10.3. Possibility of hazardous reactions
No data available.

10.4. Conditions to avoid
Excessive exposure to heat and light.

10.5. Incompatible materials
Strong oxidising agents.

10.6. Hazardous decomposition products
No known hazardous decomposition products.
11. Toxicological information

11.1. Information on toxicological effects

Acute toxicity
No data available.

Skin corrosion/irritation
No data available.

Serious eye damage/eye 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.

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available.

Aspiration hazard
No data available.

Routes of exposure
Eye contact, ingestion, inhalation, skin contact.

Signs and Symptoms of Exposure

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

12. Ecological information

12.1. Toxicity
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. Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6. Other adverse effects
No data available.
13. Disposal

13.1. Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state and local environmental regulations and directives on waste and hazardous waste. Offer surplus material to a licensed professional waste disposal professional.

Contaminated packaging
Dispose of as unused product.

14. Transport

Non-hazardous for road, air and sea transport.

IATA: Not regulated as a hazardous material.
IMO: Not regulated as a hazardous material.
RID/ADR: Not regulated as a hazardous material.

15. Regulatory information

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006, the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).

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

No data available.

15.2 Chemical safety assessment

No chemical safety report/assessment was carried out for this product.

16. Other information

Warranty
This material is for research and development use only. The information provided here is based upon the available information from material suppliers but not warranted as complete and is provided only as a guide. Ossila Limited shall not be held responsible for any damage resulting from use or handling of this product.