



Safety Data Sheet

1. IDENTIFICATION OF THE SUBSTANCES/MIXTURE AND OF THE COMPANY/UNDERTAKING

- 1.1. Product Identifiers**
- Product Code(s)** HB3717
- Product Name** 2,5-Dimethyl celecoxib
- 1.2. Relevant identified uses of the substance or mixture and uses advised against**
- Recommended use** For research use only – Not for human use
- Uses advised against** No information available
- 1.3. Details of the supplier of the safety data sheet**
- Supplier**
- HelloBio Ltd
Unit 3 IO Centre
Cabot Park
Moorend Farm Avenue
Avonmouth
Bristol
BS 11 0QL
UK
Tel: +44 (0)117 318 0505
Fax: +44 (0)1179 811 601
- For further information, please contact: technicalsupport@hellobio.com
- 1.4. Emergency Telephone number**
- Emergency telephone** - Tel: +44 (0)117 318 0505

2. HAZARDS IDENTIFICATION

- 2.1. Classification of the substance or mixture**
GHS/CLP – REGULATION (EC) No 1272/2008
- Acute oral toxicity Category 3

DSD/DPD – Classification according to EU Directives 67/548/EEC or 1999/45/EC

T - Toxic

R23/24/25 – Toxic by inhalation, in contact with skin and if swallowed

2.2. Label Elements



Signal Word

Danger

Hazard Statements

H301 – Toxic if swallowed

Precautionary Statements

P301 + P310 - IF SWALLOWED: Immediately call POISON CENTER or doctor/physician

P260 - Do not breathe dust/fume/gas/mist/vapours/pray

P262 - Do not get in eyes, on skin, or on clothing

P280 - Wear protective gloves/ eye protection/ face protection

P284 - Wear respiratory protection

P361 - Remove/Take off immediately all contaminated clothing

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

P271 - Use only outdoors or in a well-ventilated area

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

P330 - Rinse mouth

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

P405 - Store locked up

P363 - Wash contaminated clothing before use

Other hazards

Caution – substance not yet completely tested

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Product Name: 2,5-Dimethylcelecoxib

Synonyms:

Formula: $C_{18}H_{16}F_3N_3O_2S$

Molecular Weight: 395.40

CAS Number 457639-36-8

4. FIRST AID MEASURES

4.1. Description of first aid measures

General advice

If symptoms persist, call a physician.

Eye contact

Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. If symptoms persist, call a physician.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. If symptoms persist, call a physician.

Ingestion	Rinse mouth. If symptoms persist, call a physician
Inhalation	Move to fresh air. If symptoms persist, call a physician.

- 4.2. Most important symptoms and effects, both acute and delayed**
To the best of our knowledge, the chemical, physical and toxicological properties have not been thoroughly investigated.
- 4.3. Indication of immediate medical attention and special treatment needed**
Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

5. FIRE-FIGHTING 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**
In combustion, may emit toxic fumes.
- 5.3. Precautions for fire-fighters**
Wear suitable protective clothing to prevent contact with skin and eyes and self-contained breathing apparatus.

6. ACCIDENTAL RELEASE MEASURES

- 6.1. Personal precautions, protective equipment and emergency procedures**
Do not take action without suitable protective clothing – see section 8 of SDS. Evacuate personnel to safe areas. Ensure adequate ventilation. Avoid breathing vapours, mist, dust or gas.
- 6.2. Environmental precautions**
Do not let product enter drains.
- 6.3. Methods and materials for containment and cleaning up**
Cover spillage with suitable absorbent material. Using non-spark tools, sweep up material and place in an appropriate container. Decontaminate spill site with 10% caustic solution and ventilate area until disposal is complete. Hold all material for appropriate disposal as described under section 13 of SDS.
- 6.4. Reference to other sections**
For required PPE see section 8. For disposal see section 13.

7. HANDLING AND STORAGE

- 7.1. Precautions for safe handling**
Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid the formation of dust and aerosols. Use in a well-ventilated area. Keep away from sources of ignition. Avoid prolonged or repeated exposure.
- 7.2. Conditions for safe storage, including any incompatibilities.**
Store in cool, well-ventilated area. Keep away from direct sunlight. Keep container tightly sealed until ready for use. Recommended storage temperature: Store at RT
- 7.3. Specific end uses**
Use in a laboratory fume hood where possible. Refer to employer's COSHH risk assessment.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2. Exposure controls

Appropriate engineering controls

Use in a fume hood where applicable. Ensure all engineering measures described under section 7 of SDS are in place. Ensure laboratory is equipped with a safety shower and eye wash station.

Personal protective equipment

Eye/face protection

Use appropriate safety glasses.

Skin protection

Use appropriate chemical resistant gloves (minimum requirement use standard BS EN 374:2003). Gloves should be inspected before use. Wash and dry hands thoroughly after handling.

Body protection

Wear appropriate protective clothing.

Respiratory protection

If risk assessment indicates necessary, use a suitable respirator.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance	White solid	Vapour pressure	No data available
Odour	No data available	Vapour density	No data available
Odour threshold	No data available	Relative density	No data available
pH	No data available	Solubility(ies)	Dimethylsulfoxide
Melting/freezing point	No data available	Partition coefficient	No data available
Boiling point/range	No data available	Auto-ignition temperature	No data available
Flash Point	No data available	Decomposition temperature	No data available
Evaporation rate	No data available	Viscosity	No data available
Flammability (solid, gas)	No data available	Explosive properties	No data available
Upper/lower flammability or explosive limits	No data available	Oxidising properties	No data available

9.2. Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1. Reactivity

Stable under recommended transport or storage conditions.

10.2. Chemical Stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous reactions will not occur under normal transport or storage conditions.

- 10.4. Conditions to avoid**
Heat, moisture
- 10.5. Incompatible materials**
Strong acids/alkalis, strong oxidising/reducing agents.
- 10.6. Hazardous decomposition products**
Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Phosphorous oxides.

11. TOXICOLOGICAL INFORMATION

11.1. Information on toxicological effects

Acute Toxicity

Inhalation	No Information available
Eye contact	No Information available
Skin contact	No Information available
Ingestion	No Information available

Chronic toxicity

Corrosivity	No Information available
Sensitization	No Information available
Neurological effects	No Information available
Reproductive toxicity	No Information available
Mutagenic effects	No Information available
Target Organ Effects	No Information available

12. ECOLOGICAL INFORMATION

12.1. Toxicity Ecotoxicity effects

As supplied, the preparation is not expected to present significant adverse environmental effects

12.2. Persistence and degradability

No Information available

12.3. Bioaccumulative potential

No Information available

12.4. Mobility in soil

No Information available

12.5. Results of PBT and vPvB assessment

No Information available

12.6. Other adverse effects

No Information available

13. DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from residues/unused products

Dispose of in accordance with local regulations

Contaminated packaging

Empty containers should be taken to an approved waste handling site for recycling or disposal.

Other information

According to the European Waste Catalogue. Waste Codes are not product specific, but application specific. Waste codes should be assigned by the user based on the application for which the product was used.

14. TRANSPORT INFORMATION

ADR	Excepted Quantity
Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (2', 5'-dimethyl celecoxib
Hazard Class	6.1
UN/ID No	2811
Packing Group	III
IATA	Excepted Quantity
Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (2', 5'-dimethyl celecoxib
Hazard Class	6.1
UN/ID No	2811
Packing Group	III
DOT	Excepted Quantity
Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (2', 5'-dimethyl celecoxib
Hazard Class	6.1
UN/ID No	2811
Packing Group	III

15. REGULATORY INFORMATION

- 15.1. **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No information available
- 15.2. **Chemical Safety Assessment**
No information available

16. OTHER INFORMATION

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe

handling, use, processing, storage, transportation , disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless stated in the text.