SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

- **Product name:** Ibuprofen impurity B; (2RS)-2-(4-Butylphenyl)propionic acid (0,06% solution in Acetonitrile)
- **Part number:** EPB1220000

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

No further relevant information available.

1.3 Details of the supplier of the safety data sheet

- **Manufacturer/Supplier:**
  - LGC Limited
  - Queens Road
  - Teddington
  - Middlesex TW11 0LY
  - UNITED KINGDOM

- **Further information obtainable from:**
  - Product safety department
eMail: sds-request@lgcgroup.com
- **Emergency telephone number:** +44 (0) 20 8943 7000 (Monday - Friday: 8am - 5pm)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

- **Classification according to Regulation (EC) No 1272/2008**

<table>
<thead>
<tr>
<th>GHS02 flame</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flam. Liq. 2 H225</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>GHS07</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute Tox. 4 H302</td>
</tr>
<tr>
<td>Acute Tox. 4 H312</td>
</tr>
<tr>
<td>Acute Tox. 4 H332</td>
</tr>
<tr>
<td>Eye Irrit. 2 H319</td>
</tr>
</tbody>
</table>

2.2 Label elements

- **Labelling according to Regulation (EC) No 1272/2008**
  The product is classified and labelled according to the CLP regulation.

- **Hazard pictograms**

  | GHS02 | GHS07 |

- **Signal word** Danger

- **Hazard-determining components of labelling:**
  - Acetonitrile

- **Hazard statements**
  - H225: Highly flammable liquid and vapour.
  - H302+H312+H332: Harmful if swallowed, in contact with skin or if inhaled.
**Product name:** Ibuprofen impurity B; (2RS)-2-(4-Butylphenyl)propionic acid (0.06% solution in Acetonitrile)

(Contd. from page 1)

- **Precautionary statements**
  - **P210** Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
  - **P241** Use explosion-proof electrical/ventilating/lighting equipment.
  - **P280** Wear protective gloves/protective clothing/eye protection/face protection.
  - **P303+P361+P353** IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
  - **P305+P361+P338** IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
  - **P501** Dispose of contents/container in accordance with local/regional/national/international regulations.

- **2.3 Other hazards**
  - **Results of PBT and vPvB assessment**
    - **PBT:** Not applicable.
    - **vPvB:** Not applicable.

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**SECTION 3: Composition/information on ingredients**

- **3.2 Chemical characterisation: Mixtures**
  - **Description:** Mixture: consisting of the following components.

  | CAS: 75-05-8 | Acetonitrile |
  | EINECS: 200-835-2 | Flam. Liq. 2, H225; Acute Tox. 4, H302; Acute Tox. 4, H312; Acute Tox. 4, H332; Eye Irrit. 2, H319 |
  | RTECS: AL 7700000 | > 99% |

| CAS: 3585-49-7 | (2RS)-2-(4-Butylphenyl)propionic Acid |
| EC number: 641-468-1 | Acute Tox. 4, H302 |
| RTECS: - | < 0.1% |

- **Additional information:** For the wording of the listed hazard phrases refer to section 16.

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**SECTION 4: First aid measures**

- **4.1 Description of first aid measures**
  - **General information:** Symptoms of poisoning may occur even after several hours; therefore medical observation for at least 48 hours after the accident is recommended.
  - **After inhalation:** Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.
    - In case of unconsciousness place patient in recovery position for transport.
    - Seek medical treatment.
  - **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
    - Seek medical treatment.
  - **After eye contact:** Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
  - **After swallowing:** Rinse mouth. Do not induce vomiting.
    - Seek medical treatment.

- **4.2 Most important symptoms and effects, both acute and delayed** No further relevant information available.

(Contd. on page 3)
4.3 Indication of any immediate medical attention and special treatment needed
No further relevant information available.

SECTION 5: Firefighting measures

- 5.1 Extinguishing media
  - Suitable extinguishing agents:
    CO2, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

- 5.2 Special hazards arising from the substance or mixture
  - Formation of toxic gases is possible during heating or in case of fire.

- 5.3 Advice for firefighters
  - Protective equipment:
    - Mouth respiratory protective device.
    - Wear self-contained respiratory protective device.

SECTION 6: Accidental release measures

- 6.1 Personal precautions, protective equipment and emergency procedures
  - Wear protective equipment. Keep unprotected persons away.

- 6.2 Environmental precautions:
  - Dilute with plenty of water.
  - Do not allow to enter sewers/surface or ground water.

- 6.3 Methods and material for containment and cleaning up:
  - Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
  - Ensure adequate ventilation.

- 6.4 Reference to other sections
  - See Section 7 for information on safe handling.
  - See Section 8 for information on personal protection equipment.
  - See Section 13 for disposal information.

SECTION 7: Handling and storage

- 7.1 Precautions for safe handling
  - Ensure good ventilation/extraction at the workplace.
  - Store in cool, dry place in tightly closed receptacles.
  - Information about fire - and explosion protection:
    - Keep ignition sources away - Do not smoke.
    - Protect against electrostatic charges.

- 7.2 Conditions for safe storage, including any incompatibilities
  - Storage:
    - Requirements to be met by storerooms and receptacles:
      - Please refer to the manufacturer's certificate for specific storage and transport temperature conditions.
      - Store only in the original receptacle.
      - Keep container in a well-ventilated place. Keep away from sources of ignition and heat.
      - Information about storage in one common storage facility: Store away from foodstuffs.
    - Further information about storage conditions:
      - Keep container tightly sealed.
      - Store in cool, dry conditions in well sealed receptacles.

- 7.3 Specific end use(s) No further relevant information available.

(Contd. on page 4)
Product name: Ibuprofen impurity B; (2RS)-2-(4-Butylphenyl)propionic acid (0.06% solution in Acetonitrile)

SECTION 8: Exposure controls/personal protection

- Additional information about design of technical facilities: No further data; see item 7.

- Ingredients with limit values that require monitoring at the workplace:

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>WEL Short-term value</th>
<th>Long-term value</th>
</tr>
</thead>
<tbody>
<tr>
<td>75-05-8 Acetonitrile</td>
<td>102 mg/m³, 60 ppm</td>
<td>68 mg/m³, 40 ppm</td>
</tr>
</tbody>
</table>

- Additional information: Lists used were valid at the time of SDS preparation.

- 8.2 Exposure controls
- Personal protective equipment:
  - General protective and hygienic measures:
    - Keep away from foodstuffs, beverages and feed.
    - Immediately remove all soiled and contaminated clothing.
    - Wash hands before breaks and at the end of work.
    - Avoid contact with the eyes.
    - Avoid contact with the eyes and skin.
  - Respiratory protection:
    - In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.
  - Protection of hands:
    - The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
    - Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation.
    - The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374.
    - Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Protective gloves

- Material of gloves
  - The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.
  - Butyl rubber, BR

- Penetration time of glove material
  - The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection:

Tightly sealed goggles
SECTION 9: Physical and chemical properties

- 9.1 Information on basic physical and chemical properties
  - General Information
  - Appearance:
    - Form: Liquid
    - Colour: Colourless
  - Odour:
    - Aromatic
  - Odour threshold: Not determined.
  - pH-value: Not determined.
  - Change in condition
    - Melting point/freezing point: -46 °C
    - Initial boiling point and boiling range: 81 °C
  - Flash point: 5 °C
  - Flammability (solid, gas): Not determined.
  - Ignition temperature: 525 °C
  - Decomposition temperature: Not determined.
  - Auto-ignition temperature: Product is not selfigniting.
  - Explosive properties: Product is not explosive. However, formation of explosive air/vapour mixtures is possible.
    - Explosion limits: Lower: 4.4 Vol %
      Upper: 16 Vol %
    - Vapour pressure at 20 °C: 97 hPa
    - Density at 20 °C: 0.78165 g/cm³
    - Relative density: Not determined.
    - Vapour density: Not determined.
    - Evaporation rate: Not determined.
    - Solubility in / Miscibility with water at 25 °C: 74 g/l
    - Partition coefficient: n-octanol/water: Not determined.
  - Viscosity:
    - Dynamic: Not determined.
    - Kinematic: Not determined.

- 9.2 Other information
  No further relevant information available.

SECTION 10: Stability and reactivity

- 10.1 Reactivity Stable under normal conditions.
- 10.2 Chemical stability Stable under normal conditions.
- Thermal decomposition / conditions to be avoided:
  Formation of toxic gases is possible during heating or in case of fire.
- 10.3 Possibility of hazardous reactions Forms explosive gas mixture with air.
- 10.4 Conditions to avoid
  Sources of ignition
  Heat.

(Contd. on page 6)
Product name: Ibuprofen impurity B; (2RS)-2-(4-Butylphenyl)propionic acid (0.06% solution in Acetonitrile)

- 10.5 Incompatible materials:
  - Strong oxidizing agents.
  - Strong acids.
- 10.6 Hazardous decomposition products:
  Formation of toxic gases is possible during heating or in case of fire.

SECTION 11: Toxicological information

- 11.1 Information on toxicological effects
  - Acute toxicity
    - Harmful if swallowed, in contact with skin or if inhaled.

<table>
<thead>
<tr>
<th>LD/LC50 values relevant for classification:</th>
</tr>
</thead>
<tbody>
<tr>
<td>75-05-8 Acetonitrile</td>
</tr>
<tr>
<td>Oral (LD50) 2460 mg/kg (rat)</td>
</tr>
</tbody>
</table>

- Primary irritant effect:
  - Skin corrosion/irritation Based on available data, the classification criteria are not met.
  - Serious eye damage/irritation
    Causes serious eye irritation.
  - Respiratory or skin sensitisation Based on available data, the classification criteria are not met.
  - CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)
  - Germ cell mutagenicity Based on available data, the classification criteria are not met.
  - Carcinogenicity Based on available data, the classification criteria are not met.
  - Reproductive toxicity Based on available data, the classification criteria are not met.
  - STOT-single exposure Based on available data, the classification criteria are not met.
  - STOT-repeated exposure Based on available data, the classification criteria are not met.
  - Aspiration hazard Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

- 12.1 Toxicity
  - Aquatic toxicity:
    75-05-8 Acetonitrile
    | EC50/48 h | 3600 mg/l (daphnia) |
    | LC50/96 h | 1640 mg/l (fish) |

- 12.2 Persistence and degradability
  - No further relevant information available.
- 12.3 Bioaccumulative potential
  - No further relevant information available.
- 12.4 Mobility in soil
  - No further relevant information available.
- Additional ecological information:
  - General notes:
    Water hazard class 2 (German Regulation) (Self-assessment): hazardous for water
    Do not allow product to reach ground water, water course or sewage system.
    Danger to drinking water if even small quantities leak into the ground.
  - 12.5 Results of PBT and vPvB assessment
    - PBT: Not applicable.
    - vPvB: Not applicable.
  - 12.6 Other adverse effects
    - No further relevant information available.
Product name: Ibuprofen impurity B; (2RS)-2-(4-Butylphenyl)propionic acid (0.06% solution in Acetonitrile)

SECTION 13: Disposal considerations

- 13.1 Waste treatment methods
- Recommendation
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- European waste catalogue
Waste disposal key numbers from EWC have to be assigned depending on origin and processing.

- Uncleaned packaging:
- Recommendation: Dispose of in accordance with national regulations.
- Recommended cleansing agents: Water, if necessary together with cleansing agents.

SECTION 14: Transport information

- 14.1 UN-Number
- ADR, IMDG, IATA UN1648
- ADR 1648 ACETONITRILE mixture
- IMDG, IATA ACETONITRILE mixture

- 14.3 Transport hazard class(es)
- ADR, IMDG, IATA
**Class** 3 Flammable liquids.
**Label** 3

- 14.4 Packing group
- ADR, IMDG, IATA II

- 14.5 Environmental hazards:
- Marine pollutant: No

- 14.6 Special precautions for user
- Warning: Flammable liquids.
- Danger code (Kemler): 33
- EMS Number: F-E-S-D
- Stowage Category B
- Stowage Code SW2 Clear of living quarters.

- 14.7 Transport in bulk according to Annex II of Marpol and the IBC Code
- Not applicable.

- Transport/Additional information:

- ADR
- Excepted quantities (EQ): E2
- Limited quantities (LQ): 1L
- Transport category 2
- Tunnel restriction code D/E
- UN "Model Regulation": UN 1648 ACETONITRILE MIXTURE, 3, II

(Contd. on page 8)
**Product name:** Ibuprofen impurity B; (2RS)-2-(4-Butylphenyl)propionic acid (0.06% solution in Acetonitrile)

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**SECTION 15: Regulatory information**

- **15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
  - **Philippines Inventory of Chemicals and Chemical Substances**
    - 75-05-8 Acetonitrile
  - **Australian Inventory of Chemical Substances**
    - 75-05-8 Acetonitrile
  - **Standard for the Uniform Scheduling of Medicines and Poisons**
    - None of the ingredients is listed.

  - **Directive 2012/18/EU**
  - **Named dangerous substances - ANNEX I** None of the ingredients is listed.
  - **Seveso category P5c FLAMMABLE LIQUIDS**
  - **Qualifying quantity (tonnes) for the application of lower-tier requirements** 5.000 t
  - **Qualifying quantity (tonnes) for the application of upper-tier requirements** 50.000 t
  - **REGULATION (EC) No 1907/2006 ANNEX XVII** Conditions of restriction: 3

- **15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

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**SECTION 16: Other information**

The information in this safety data sheet (SDS) has been prepared with due care and is true and accurate to the best of our knowledge. The user must determine the suitability of the information for its particular purpose, ensure compliance with existing laws and regulations, and be aware that other or additional safety or performance considerations may arise when using, handling and/or storing the material. The information in this SDS does not purport to be all inclusive or a guarantee as to the properties of the material supplied, and should be used only as a guide. LGC makes no warranties or representations as to the accuracy and completeness of the information contained herein, shall not be held responsible for the suitability of this information for the user's intended purposes or the consequences of such use, and shall not be liable for any damage or loss, howsoever arising, direct or otherwise.

- **Abbreviations and acronyms:**
  - RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
  - ICAO: International Civil Aviation Organisation
  - ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
  - IMDG: International Maritime Code for Dangerous Goods
  - IATA: International Air Transport Association
  - GHS: Globally Harmonised System of Classification and Labelling of Chemicals
  - EINECS: European Inventory of Existing Commercial Chemical Substances
  - ELINCS: European List of Notified Chemical Substances
  - CAS: Chemical Abstracts Service (division of the American Chemical Society)
  - LC50: Lethal concentration, 50 percent
  - LD50: Lethal dose, 50 percent
  - PBT: Persistent, Bioaccumulative and Toxic
  - vPvB: very Persistent and very Bioaccumulative
  - Flam. Liq. 2: Flammable liquids – Category 2
  - Eye Irrit. 2: Serious eye damage/eye irritation – Category 2

- **Sources**
  - Data compared to the previous version altered, All sections have been updated.