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

- **Product identifier**
- **Trade name:** 4-Isopropyltoluene
- **Part number:** RAB-042
- **CAS Number:** 99-87-6
- **EC number:** 202-796-7
- **Relevant identified uses of the substance or mixture and uses advised against**
  Reagents and Standards for Analytical Chemical Laboratory Use
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
  Agilent Technologies Manufacturing GmbH & Co. KG
  Hewlett-Packard-Str.8
  76337 Waldbronn
  Germany
- **Further information obtainable from:**
  Telephone: 0800 603 1000
  pdl-msds_author@agilent.com
- **Emergency telephone number:** CHEMTREC®: +(44)-870-8200418

2 Hazards identification

- **Classification of the substance or mixture**
- **Classification according to Regulation (EC) No 1272/2008**
  - GHS02 flame
  - Flam. Liq. 3 H226 Flammable liquid and vapour.
  - GHS08 health hazard
  - Asp. Tox. 1 H304 May be fatal if swallowed and enters airways.
  - GHS09 environment
  - Aquatic Chronic 2 H411 Toxic to aquatic life with long lasting effects.

- **Label elements**
- **Labelling according to Regulation (EC) No 1272/2008**
  The substance is classified and labelled according to the CLP regulation.
- **Hazard pictograms**
  - GHS02
  - GHS08
  - GHS09

(Contd. on page 2)
Signal word: Danger

Hazard-determining components of labelling:
- p-cymene

Hazard statements:
- H226 Flammable liquid and vapour.
- H304 May be fatal if swallowed and enters airways.
- H411 Toxic to aquatic life with long lasting effects.

Precautionary statements:
- P101 If medical advice is needed, have product container or label at hand.
- P102 Keep out of reach of children.
- P103 Read label before use.
- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
- P233 Keep container tightly closed.
- P240 Ground/bond container and receiving equipment.
- P241 Use explosion-proof electrical/ventilating/lighting equipment.
- P242 Use only non-sparking tools.
- P243 Take precautionary measures against static discharge.
- P273 Avoid release to the environment.
- P280 Wear protective gloves/protective clothing/eye protection/face protection.
- P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
- P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
- P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
- P370+P378 In case of fire: Use for extinction: CO2, powder or water spray.
- P391 Collect spillage.
- P403+P235 Store in a well-ventilated place. Keep cool.
- P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

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

3 Composition/information on ingredients

- Chemical characterisation: Substances
- CAS No. Description
  - 99-87-6 p-cymene
- Identification number(s)
  - EC number: 202-796-7

4 First aid measures

- Description of first aid measures
- General information: Immediately remove any clothing soiled by the product.
- After inhalation: Supply fresh air; consult doctor in case of complaints.
- After skin contact: Immediately rinse with water.
- After eye contact: Rinse opened eye for several minutes under running water.
- After swallowing: If symptoms persist consult doctor.
48.1.26 Information for doctor:

· Most important symptoms and effects, both acute and delayed: No further relevant information available.

· Indication of any immediate medical attention and special treatment needed: No further relevant information available.

5 Firefighting measures

· Extinguishing media

· Suitable extinguishing agents:
  CO2, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

· For safety reasons unsuitable extinguishing agents: Water with full jet

· Special hazards arising from the substance or mixture: No further relevant information available.

· Advice for firefighters

· Protective equipment: No special measures required.

6 Accidental release measures

· Personal precautions, protective equipment and emergency procedures

  Wear protective equipment. Keep unprotected persons away.

· Environmental precautions:

  Do not allow product to reach sewage system or any water course.
  Inform respective authorities in case of seepage into water course or sewage system.
  Do not allow to enter sewers/ surface or ground water.

· Methods and material for containment and cleaning up:

  Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
  Dispose contaminated material as waste according to item 13.
  Ensure adequate ventilation.

· 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.

7 Handling and storage

· Handling:

· Precautions for safe handling: No special precautions are necessary if used correctly.

· Information about fire - and explosion protection:

  Keep ignition sources away - Do not smoke.
  Protect against electrostatic charges.

· Conditions for safe storage, including any incompatibilities

· Storage:

  · Requirements to be met by storerooms and receptacles: No special requirements.
  · Information about storage in one common storage facility: Not required.
  · Further information about storage conditions: Keep container tightly sealed.
  · Specific end use(s) No further relevant information available.
8 Exposure controls/personal protection

- Additional information about design of technical facilities: No further data; see item 7.
- Control parameters
- Ingredients with limit values that require monitoring at the workplace: Not required.
- Additional information: The lists valid during the making were used as basis.

- 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.
- Respiratory protection:
  When used as intended with Agilent instruments the use of the product under normal laboratory conditions and
  with standard practices does not result in significant airborne exposures and therefore respiratory protection is not
  needed.
  Under an emergency condition where a respirator is deemed necessary, use a NIOSH or equivalent approved
  device equipment with appropriate organic or acid gas cartridge.
- Protection of hands:
  Although not recommended for constant contact with the chemicals or for clean up, nitrile gloves 11-13mil
  thickness are recommended for normal use. The breakthrough time is 1hr. For cleaning a spill where there is direct
  contact of the chemical, butyl rubber gloves are recommended 12-15mil thickness with breakthrough times
  exceeding 4 hrs. Supplier recommendations should be followed.
- Material of gloves
  For normal use: nitrile rubber, 11-13 mil thickness
  For direct contact with the chemical: butyl rubber, 12-15 mil thickness
  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.
- Penetration time of glove material
  For normal use: nitrile rubber: 1 hour
  For direct contact with the chemical: butyl rubber: > 4 hours
- Eye protection:

Tightly sealed goggles

9 Physical and chemical properties

- Information on basic physical and chemical properties
- General Information
- Appearance:
  Form: Fluid
  Colour: Colourless
- Odour: Characteristic
- Odour threshold: Not determined.
- pH-value: Not determined.
48.1.26

- Change in condition
  - Melting point/freezing point: -68 °C
  - Initial boiling point and boiling range: 177 °C
- Flash point: 47 °C
- Flammability (solid, gas): Not applicable.
- Ignition temperature: 435 °C
- Decomposition temperature: Not determined.
- Auto-ignition temperature: Not determined.
- Explosive properties: Product is not explosive. However, formation of explosive air/vapour mixtures are possible.
- Explosion limits:
  - Lower: 0.7 Vol %
  - Upper: 5.6 Vol %
- Vapour pressure at 20 °C: 1.5 hPa
- Density at 20 °C: 0.86 g/cm³
- Relative density: Not determined.
- Vapour density: Not determined.
- Evaporation rate: Not determined.
- Solubility in / Miscibility with water: Not miscible or difficult to mix.
- Partition coefficient: n-octanol/water: Not determined.
- Viscosity:
  - Dynamic: Not determined.
  - Kinematic: Not determined.
- Solvent content:
  - Organic solvents: 100.0 %
  - VOC (EC): 100.00 %
- Other information: No further relevant information available.

10 Stability and reactivity

- Reactivity: No further relevant information available.
- Chemical stability
- Thermal decomposition / conditions to be avoided: No decomposition if used according to specifications.
- Possibility of hazardous reactions: No dangerous reactions known.
- Conditions to avoid: No further relevant information available.
- Incompatible materials: No further relevant information available.
- Hazardous decomposition products: No dangerous decomposition products known.

(Contd. on page 6)
11 Toxicological information

- **Information on toxicological effects**
  - **Acute toxicity** Based on available data, the classification criteria are not met.
  - **LD/LC50 values relevant for classification:**
    - 99-87-6 p-cymene
    - Oral LD50 4,750 mg/kg (rat)

- **Primary irritant effect:**
  - **Skin corrosion/irritation** Based on available data, the classification criteria are not met.
  - **Serious eye damage/irritation** Based on available data, the classification criteria are not met.
  - **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**
    May be fatal if swallowed and enters airways.

12 Ecological information

- **Toxicity**
  - **Aquatic toxicity:** No further relevant information available.
  - **Persistence and degradability** No further relevant information available.
  - **Behaviour in environmental systems:**
    - **Bioaccumulative potential** No further relevant information available.
  - **Mobility in soil** No further relevant information available.
  - **Ecotoxic effects:**
  - **Remark:** Toxic for fish
  - **Additional ecological information:**
  - **General notes:**
    Water hazard class 1 (German Regulation) (Assessment by list): slightly hazardous for water
    Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
    Also poisonous for fish and plankton in water bodies.
    Toxic for aquatic organisms
  - **Results of PBT and vPvB assessment**
    - **PBT:** Not applicable.
    - **vPvB:** Not applicable.
  - **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**
  - **Recommendation**
    Must not be disposed together with household garbage. Do not allow product to reach sewage system.

- **European waste catalogue**
  - **HP 3** Flammable
### 14 Transport information

- **UN-Number**
  - ADR, IMDG, IATA
  - UN2046

- **UN proper shipping name**
  - ADR
    - 2046 CYMENES, ENVIRONMENTALLY HAZARDOUS
  - IMDG
    - CYMENES, MARINE POLLUTANT
  - IATA
    - CYMENES

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

- **IATA**
  - Class
    - 3 Flammable liquids.
  - Label
    - 3

- **Packing group**
  - ADR, IMDG, IATA
    - III

- **Environmental hazards:**
  - Marine pollutant:
    - Symbol (fish and tree)
  - Special marking (ADR):
    - Symbol (fish and tree)

- **Special precautions for user**
  - Danger code (Kemler):
    - 30
  - EMS Number:
    - 3-07
  - Stowage Category:
    - A

- **Transport in bulk according to Annex II of Marpol and the IBC Code**
  - Not applicable.
Trade name: 4-Isopropyltoluene

15 Regulatory information

- Safety, health and environmental regulations/legislation specific for the substance or mixture
- Directive 2012/18/EU
- Named dangerous substances - ANNEX I Substance is not listed.
- Seveso category
  - E2 Hazardous to the Aquatic Environment
  - P5c FLAMMABLE LIQUIDS
- Qualifying quantity (tonnes) for the application of lower-tier requirements: 200 t
- Qualifying quantity (tonnes) for the application of upper-tier requirements: 500 t
- REGULATION (EC) No 1907/2006 ANNEX XVII Conditions of restriction: 3
- Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

The information contained in this document is based on Agilent’s state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.

- Department issuing SDS: Document Control / Regulatory
- Contact: regulatory@ultrasci.com
- Abbreviations and acronyms:
  - 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
  - CAS: Chemical Abstracts Service (division of the American Chemical Society)
  - VOC: Volatile Organic Compounds (USA, EU)
  - LC50: Lethal concentration, 50 percent
  - LD50: Lethal dose, 50 percent
  - PBT: Persistent, Bioaccumulative and Toxic
  - vPvB: very Persistent and very Bioaccumulative
  - Flam. Liq. 3: Flammable liquids – Category 3
  - Asp. Tox. 1: Aspiration hazard – Category 1
  - Aquatic Chronic 2: Hazardous to the aquatic environment - long-term aquatic hazard – Category 2