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

- **Product identifier**

- **Trade name:** Pentachloronitrobenzene (Quintozene) Standard (1X1 mL)
- **Part number:** PST-770A100A01

- **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. 2  H225  Highly flammable liquid and vapour.

  - GHS07
    Acute Tox. 4  H302  Harmful if swallowed.
    Eye Irrit. 2  H319  Causes serious eye irritation.

  - **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  Harmful if swallowed.
  H319  Causes serious eye irritation.

(Contd. on page 2)
Trade name: Pentachloronitrobenzene (Quintozene) Standard (1X1 mL)

- **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.
  - P264 Wash thoroughly after handling.
  - P270 Do not eat, drink or smoke when using this product.
  - P280 Wear protective gloves/protective clothing/eye protection/face protection.
  - P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
  - P330 Rinse mouth.
  - P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
  - P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
  - P337+P313 If eye irritation persists: Get medical advice/attention.
  - P370+P378 In case of fire: Use for extinction: CO2, powder or water spray.
  - 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: Mixtures**
  - **Description:** Mixture of substances listed below with nonhazardous additions.

- **Dangerous components:**
  - CAS: 75-05-8
  - EINECS: 200-835-2
  - acetonitrile
  - 99.987%
  - Flam. Liq. 2, H225; Acute Tox. 4, H302; Acute Tox. 4, H312; Acute Tox. 4, H332; Eye Irrit. 2, H319

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

### 4 First aid measures

- **Description of first aid measures**
- **General information:**
  - Immediately remove any clothing soiled by the product.
  - Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
- **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. If symptoms persist, consult a doctor.

(Contd. on page 3)
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 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: Store in a cool location.
    - Information about storage in one common storage facility: Not required.
    - Further information about storage conditions:
      - Keep container tightly sealed.
      - Store in cool, dry conditions in well sealed receptacles.
- 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

<table>
<thead>
<tr>
<th>Ingredients with limit values that require monitoring at the workplace:</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>75-05-8 acetonitrile</strong></td>
</tr>
<tr>
<td>WEL</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

· 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.
  Avoid contact with the eyes.
  Avoid contact with the eyes and skin.

· 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

· 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
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Odour</td>
<td>Aromatic</td>
</tr>
<tr>
<td>Odour threshold</td>
<td>Not determined.</td>
</tr>
<tr>
<td>pH-value</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Change in condition</td>
<td></td>
</tr>
<tr>
<td>Melting point/freezing point</td>
<td>-46 °C</td>
</tr>
<tr>
<td>Initial boiling point and boiling range</td>
<td>81 °C</td>
</tr>
<tr>
<td>Flash point</td>
<td>2 °C</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Ignition temperature</td>
<td>525 °C</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
<td>Product is not selfigniting.</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>Product is not explosive. However, formation of explosive air/vapour mixtures are possible.</td>
</tr>
<tr>
<td>Explosion limits</td>
<td></td>
</tr>
<tr>
<td>Lower</td>
<td>4.4 Vol %</td>
</tr>
<tr>
<td>Upper</td>
<td>16 Vol %</td>
</tr>
<tr>
<td>Vapour pressure at 20 °C</td>
<td>0 hPa</td>
</tr>
<tr>
<td>Density at 20 °C</td>
<td>0.78612 g/cm³</td>
</tr>
<tr>
<td>Relative density</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Vapour density</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Solubility in / Miscibility with water</td>
<td>Not miscible or difficult to mix.</td>
</tr>
<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Viscosity</td>
<td></td>
</tr>
<tr>
<td>Dynamic at 20 °C</td>
<td>0.39 mPas</td>
</tr>
<tr>
<td>Kinematic</td>
<td>Not determined.</td>
</tr>
<tr>
<td>Solvent content</td>
<td></td>
</tr>
<tr>
<td>VOC (EC)</td>
<td>0.00 %</td>
</tr>
<tr>
<td>Solids content</td>
<td>0.0 %</td>
</tr>
<tr>
<td>Other information</td>
<td>No further relevant information available.</td>
</tr>
</tbody>
</table>

**10 Stability and reactivity**

- **Reactivity**: No further relevant information available.
- **Chemical stability**: Not applicable.
- **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.
11 Toxicological information

- Information on toxicological effects
  - Acute toxicity
    Harmful if swallowed.

<table>
<thead>
<tr>
<th>LD/LC50 values relevant for classification:</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>ATE (Acute Toxicity Estimates)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral LD50</td>
</tr>
</tbody>
</table>

75-05-8 acetonitrile

<table>
<thead>
<tr>
<th>Oral</th>
<th>LD50</th>
<th>1,320 mg/kg (rat)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dermal</td>
<td>LD50</td>
<td>&gt;2,000 mg/kg (rabbit)</td>
</tr>
<tr>
<td>Inhalative</td>
<td>LC50/4 h</td>
<td>3,587 mg/L (mouse)</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.
  - 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.

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.
  - 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.
  - 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
  HP 4 Irritant - skin irritation and eye damage
  HP 6 Acute Toxicity

- Uncleaned packaging:
  - Recommendation: Disposal must be made according to official regulations.

14 Transport information

- Not Regulated, De minimus Quantities

- UN-Number
  - ADR, IMDG, IATA UN1648

- UN proper shipping name
  - ADR 1648 ACETONITRILE solution
  - IMDG, IATA ACETONITRILE solution

- Transport hazard class(es)
  - ADR, IMDG, IATA

  - Class 3 Flammable liquids.
  - Label 3

- Packing group
  - ADR, IMDG, IATA II

- Environmental hazards:
  - Not applicable.

- Special precautions for user
  - Warning: Flammable liquids.
  - Danger code (Kemler): 33
  - EMS Number: F-E,S-D
  - Stowage Category B

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

- Transport/Additional information:
  - ADR
  - Limited quantities (LQ) 1L
Trade name: Pentachloronitrobenzene (Quintozene) Standard (1X1 mL)

- **Excepted quantities (EQ)**
  - Code: E2
  - Maximum net quantity per inner packaging: 30 ml
  - Maximum net quantity per outer packaging: 500 ml

- **Transport category**
  - 2
  - Tunnel restriction code: D/E

- **IMDG**
  - 1L
  - Code: E2
  - Maximum net quantity per inner packaging: 30 ml
  - Maximum net quantity per outer packaging: 500 ml

- **UN "Model Regulation":**
  - UN 1648 ACETONITRILE SOLUTION, 3, II

**15 Regulatory information**

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
  - 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
  - **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.

- **Relevant phrases**
  - H225 Highly flammable liquid and vapour.
  - H302 Harmful if swallowed.
  - H312 Harmful in contact with skin.
  - H319 Causes serious eye irritation.
  - H332 Harmful if inhaled.

- **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
  - ELINCS: European List of Notified 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. 2: Flammable liquids – Category 2
  - Acute Tox. 4: Acute toxicity – Category 4
  - Eye Irrit. 2: Serious eye damage/eye irritation – Category 2