DATA SHEET Nr 2680 F

4-tert-BUTYLCYCLOHEXYL CHLOROFORMATE
PTBCCF

SYNONYM
Carbonochloridic acid, 4(1,1-dimethyl ethyl) cyclohexyl ester.

APPEARANCE
Clear liquid with pungent odor.

PHYSICAL PROPERTIES
Density (20 °C): 1.04 g/cm³
Boiling point: starts to decompose at 50 °C
Melting point: (-20) - (-10) °C
Solubility:
Soluble in usual organic solvents (acetone, toluene, chloroform, THF).

CHEMICAL PROPERTIES
- Reacts by hydrolysis yielding hydrochloric acid and 4-tert-butylcyclohexanol.
- Reacts with alcohols yielding carbonates.
- Reacts with amines yielding carbamates.

USES
- Organic synthesis intermediate.

Molecular formula: C₁₁H₁₉ClO₂
Molecular weight: 218.6
CAS number: 42125-46-2
EC number: 255-670-9
4-tert-BUTYLCYCLOHEXYL CHLOROFORMATE
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SPECIFICATION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Guaranteed value</th>
<th>Method</th>
<th>Operating procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Clear liquid</td>
<td>Visual</td>
<td></td>
</tr>
<tr>
<td>Color</td>
<td>≤ 50 APHA</td>
<td>Colorimetry</td>
<td>C – 210</td>
</tr>
<tr>
<td>Assay</td>
<td>≥ 97.0 %</td>
<td>Acidimetry</td>
<td>A – 245</td>
</tr>
<tr>
<td>Phosgene + hydrogen chloride</td>
<td>≤ 0.05 %</td>
<td>Iodometry+Acidimetry</td>
<td>I – 230 + A – 220</td>
</tr>
<tr>
<td>Carbon tetrachloride</td>
<td>≤ 0.03 %</td>
<td>Gas chromatography</td>
<td>GC – 395</td>
</tr>
<tr>
<td>Iron</td>
<td>≤ 1 ppm</td>
<td>Atomic absorption spectrometry</td>
<td>AAS – 810</td>
</tr>
</tbody>
</table>

PACKAGING
IBC containing 1000 kg.

HANDLING PRECAUTIONS
- Physicochemical hazard:
  Flash point (closed cup): 64 °C
- Health hazards:
  LD 50 (oral, rat): 4660 mg/kg
  Slightly irritating on skin, mucous membrane and eyes. Corrosive.
- Recommended:
  Avoid contact with metallic compounds (especially iron salts) which catalyze its decomposition.
  When handling this product wear gloves, goggles, mask and protective clothes.
  If eyes or skin are contaminated wash immediately with clean water for at least 15 minutes. In case of inhalation of concentrated vapors take person to fresh air. In both cases consult a physician.
- Neutralization:
  Neutralize by reaction with an alkaline solution.

STORAGE
Keep in its original, closed and labelled container. The place of storage has to be properly ventilated and cleanable.

Store in dry place, storage temperature must be:
< 0°C
In contact with metallic compounds it decomposes yielding hydrogen chloride and carbon dioxide and the inner pressure of the drum increases, therefore it has to be opened with care.
In case of prolonged storage it is recommended to check again the product before use by measuring typical parameters of its quality such as color, hydrogen chloride and 4-tert-butylcyclohexanol levels.

TRANSPORTATION
Refrigerated transport.
Refer to MSDS.