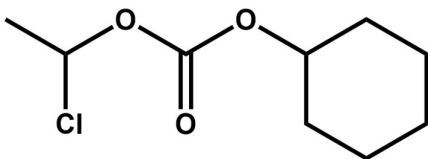


DATA SHEET Nr 3600 J

1-CHLOROETHYL CYCLOHEXYL CARBONATE

1CECC



Molecular formula: $C_9H_{15}ClO_3$

Molecular weight: 206.7

CAS number: 99464-83-2

EC number: 444-950-8

SYNONYM

Carbonic acid, 1-chloroethyl cyclohexyl ester
Cilexetil chloride

APPEARANCE

Clear liquid with pungent odor

PHYSICAL PROPERTIES

Density: 1.12 g/cm³
Melting point: -16 °C
Boiling Point: 184 °C (pred.)

Solubility:

Soluble in common organic solvents (toluene, acetone, chloroform, THF).

CHEMICAL PROPERTIES

- Slowly hydrolyzes to its constitutive alcohols and carbonic acid

USES

- Useful building block in a range of pharmaceutical syntheses
- Frequently used to functionalize pharmaceutical intermediates with pendant cyclohexyl carbonate moieties.

1-CHLOROETHYL CYCLOHEXYL CARBONATE (1CECC)

SPECIFICATION

| Parameter | Guaranteed value | Method | Operating procedure |
|----------------------------|-----------------------------|--------------------|---------------------|
| Appearance | Clear liquid | Visual control | |
| Colour | from colorless to yellowish | Visual control | |
| HCl | ≤ 0,01 % | Acidimetry | A-220 |
| Purity | ≥ 98,0 % | Gas chromatography | GC-390 |
| Dicyclohexyl carbonate | ≤ 0,2 % | Gas chromatography | GC-390 |
| Cyclohexanol | ≤ 1,0 % | Gas chromatography | GC-390 |
| I1 impurity | ≤ 0,05 % | Gas chromatography | GC-390 |
| I2 impurity | ≤ 0,05 % | Gas chromatography | GC-390 |
| I3 impurity | ≤ 0,2 % | Gas chromatography | GC-390 |
| Unspecified impurity, each | ≤ 0,2 % | Gas chromatography | GC-390 |
| Water | ≤ 0,05 % | Karl-Fischer | K-110 |

PACKAGING

PE drum containing 220 kg.

PE-lined metal drum containing 200 kg.

HANDLING PRECAUTIONS

- Physical chemical hazard: Flashpoint (tag close cup): 100 °C
- Health hazards:
LD 50 (rat, oral): 5600 mg/kg.
Irritating on skin, mucous membranes and eyes.

- Recommended:

When handling, wear approved safety eyewear, chemical resistant gloves and laboratory-appropriate protective clothing

For contact with skin or eyes, flush the contaminated area for at least 15 minutes with clean water and contact a physician.

For acute inhalation, remove the person to fresh air immediately and contact a physician.

Destruction by incineration.

STORAGE

Stored in its closed original drum in a covered, dry and well-ventilated area below 15°C the product is stable.

In the case of prolonged storage, the product should be re-analyzed for the existence of chemical degradation (coloration, cyclohexanol).

TRANSPORT

Refer to MSDS.