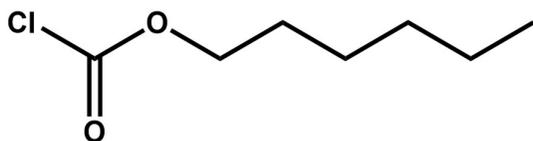


DATA SHEET Nr 2350 H
n-HEXYL CHLOROFORMATE
NHEXCF



Molecular formula: C₇H₁₃ClO₂

Molecular weight: 164.6

CAS number: 6092-54-2

EC number: 228-036-4

SYNONYMS

Chlorocarbonic acid, n-hexyl ester
n-Hexyl chlorocarbonate
Hexyloxycarbonyl chloride

APPEARANCE

Clear liquid with pungent odor.

PHYSICAL PROPERTIES

Density (20 °C): 1.01 g/cm³

Boiling point: 60 °C (1 kPa)

Solubility:

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

CHEMICAL PROPERTIES

- Reacts by hydrolysis to yield hydrochloric acid, hexanol and carbon dioxide.
- Reacts with amines yielding n-hexyl carbamates
- Reacts with alcohols to yield n-hexyl carbonates.

USES

- Used for derivatization of analytes in chromatographic analysis
- Component in the syntheses of asymmetric carbonates utilized as solvents and battery electrolyte materials
- Used as a building block in a range of pharmacological syntheses frequently involving n-hexyl carbonates or carbamate functionalities

n-HEXYL CHLOROFORMATE NHEXCF

SPECIFICATION

| Parameter | Guaranteed value | Method | Operating procedure |
|----------------------------|------------------|--------------------|---------------------|
| Appearance | Clear liquid | Visual | |
| Color | ≤ 50 APHA | Colorimetry | C – 210 |
| Assay | ≥ 98.0 % | Acidimetry | A – 245 |
| Purity | ≥ 99.0 % | Gas chromatography | GC – 168 |
| 2-Ethylbutyl chloroformate | ≤ 0.10 % | Gas chromatography | GC – 168 |
| 2-Heptyl chloroformate | ≤ 0.15 % | Gas chromatography | GC – 168 |
| 1-Octyl chloroformate | ≤ 0.10 % | Gas chromatography | GC – 168 |
| Undecane | ≤ 0.15 % | Gas chromatography | GC – 168 |
| 3-Octanol | ≤ 0.15 % | Gas chromatography | GC – 168 |
| 1-Chlorohexane | ≤ 0.15 % | Gas chromatography | GC – 168 |
| 3-Chlorohexane | ≤ 0.15 % | Gas chromatography | GC – 168 |
| Methyl chloroformate | ≤ 0,05 % | Gas chromatography | GC – 168 |
| Dihexyl carbonate | ≤ 0.20 % | Gas chromatography | GC – 168 |
| Any unspecified impurity | ≤ 0.10 % | Gas chromatography | GC – 168 |
| Sum of the impurities | ≤ 1.0 % | Gas chromatography | GC – 168 |

PACKAGING

Polyethylene lined metal drum containing 190 kg.
Polyethylene lined metal drum containing 50 kg.

HANDLING PRECAUTIONS

- Physicochemical hazard:
Flash point (closed cup): 69 °C
- Health hazards:
LC 50 (inhalation, rat): 1.17 mg/l/4h

Corrosive; irritating to skin, mucous membranes and eyes

- Recommended:
Avoid contact with metals that catalyze decomposition.

Approved safety eyewear, chemically resistant gloves and laboratory-appropriate chemical resistant clothing are recommended when handling

In case of contact with eyes, flush for a minimum of 15 minutes with fresh water and contact a physician.

In case of acute inhalation, remove the contaminated individual to fresh air and seek medical assistance.

- Neutralization:
Neutralize by reaction with cold alkaline solutions.

STORAGE

The product is stable if stored in its closed original drum in a covered, dry, cool and well-ventilated area.

In the case of prolonged storage, re-analyze for the presence of HCl and butanol prior to use

TRANSPORTATION

Refer to MSDS

Nr 2350 H

August 2018



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