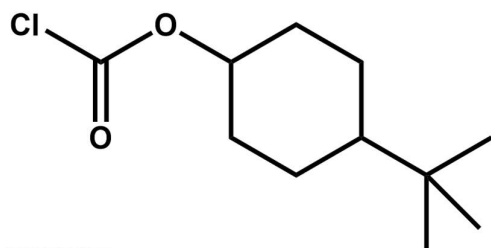


DATA SHEET Nr 2680 F

4-tert-BUTYLCYCLOHEXYL CHLOROFORMATE

PTBCCF



Molecular formula :	C ₁₁ H ₁₉ ClO ₂
Molecular weight	218.6
CAS number:	42125-46-2
EC number:	255-670-9

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 to -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 4-tert-butylcyclohexyl carbonates.
- Reacts with amines yielding 4-tert-butylcyclohexyl carbamates.

USES

- Building block in pharmaceutical syntheses
- Precursor for several known fragrance compounds
- Precursor to peroxy-type polymerization initiators

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SPECIFICATION

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

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: $< 0^{\circ}\text{C}$

In contact with metallic compounds it decomposes yielding hydrogen chloride and carbon dioxide and the inner pressure of the drum increases. Take care when opening.

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.

Nr 2680 F August 2018