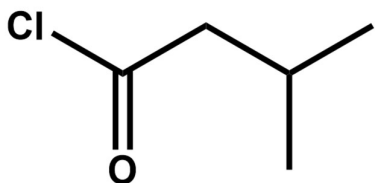


DATA SHEET Nr 1631 A
ISOVALERYL CHLORIDE
IVACL



Molecular formula: C₅H₉ClO

Molecular weight: 120.6

CAS number: 180-12-3

EC number: 203-522-2

SYNONYMS

3-Methyl butyryl chloride

Isopentanoyl chloride

Isovaleroyl chloride

APPEARANCE

Clear liquid with pungent odor.

PHYSICAL PROPERTIES

Density (20 °C): 0.989 g/cm³

Boiling point: 117 °C/101 kPa

Solubility:

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

CHEMICAL PROPERTIES

- Reacts by hydrolysis to yield hydrochloric acid and isovaleric acid
- Reacts with amines to yield isopentanamides.
- Reacts with alcohols to yield isopentanoates.

USES

- Used as a building block to deliver isopentyl ester or amide moieties in a range of pharmacological syntheses

ISOVALERYL CHLORIDE IVACL

SPECIFICATION

Parameter	Guaranteed value	Method	Operating procedure
Appearance	Clear liquid	Visual	
Color	≤ 50 APHA	Colorimetry	C – 210
Purity	≥ 98 %	Gas chromatography	GC – 544
Phosgene	≤ 0.1 %	Iodometry	I – 230
Acidity (HCl)	≤ 0.1 %	Acidimetry	A – 220

PACKAGING

Polyethylene drum containing 190 kg or PE lined metal drum 180 kg.

HANDLING PRECAUTIONS

- Physicochemical hazard:
Flash point (closed cup): 27 °C

- Health hazards:
LD 50 (oral, rat): 545 mg/kg

Corrosive; irritating to skin, mucous membranes and eyes

- Recommended:

Avoid contact with metallic compounds, especially iron, as these 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.

However, in case of prolonged storage it is recommended to re-analyze for valeric acid and HCl.

TRANSPORTATION

Refer to MSDS

Nr 1631 A

January 2022



503/0113(7)-465(7)