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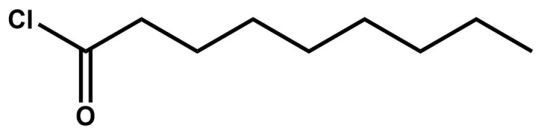
DATA SHEET Nr 1100 F

OCTANOYL CHLORIDE

NOCL



Molecular formula: $C_8H_{15}ClO$
Molecular weight: 162.7
CAS number: 111-64-8
EC number: 203-81-6

SYNONYMS

Capryloyl chloride
Octanoic acid chloride
Octanoic chloride

APPEARANCE

Clear liquid with pungent odor.

PHYSICAL PROPERTIES

Density (20 °C):	0.95 g/cm^3
Melting point:	−63 °C
Boiling point:	196 °C/101 kPa

Solubility:

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

CHEMICAL PROPERTIES

- Reacts by hydrolysis to yield hydrochloric acid and octanoic acid.
- Reacts with amines to yield octanyl amides.
- Reacts with alcohols to yield octanoates.

USES

- Used in the production of polymerization initiators.
- Useful for augmenting the aqueous solubility of functionalized compounds, imparting hydrophobicity or surfactant qualities
- Has been used to functionalize acene-type compounds for use in organic semiconductors and thin film transistors

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SPECIFICATION

Parameter	Guaranteed value	Method	Operating procedure
Appearance	Clear liquid	Visual	
Color	≤ 50 APHA	Colorimetry	C – 210
Purity	≥ 99.0 %	Gas chromatography	GC – 422
C_6 chlorides	≤ 0.5 %	Gas chromatography	GC – 422
C_{10} chlorides	≤ 0.5 %	Gas chromatography	GC – 422
Phosgene	≤ 0.1 %	Iodometry	I – 230
Acidity (HCl)	≤ 0.1 %	Acidimetry	A – 220
Octanoic acid	≤ 0.1 %	Gas chromatography	GC – 422
Other chlorides (each)	≤ 0.1 %	Gas chromatography	GC – 422
Octanoic anhydride	≤ 1.0 %	Gas chromatography	GC – 422

PACKAGING

Polyethylene lined metal drum containing 180 kg.
Polyethylene drum containing 195 kg.
In bulk.

HANDLING PRECAUTIONS

- Physicochemical hazard:
  Flash point (closed cup): 82 °C

- Health hazards:
  LD 50 (oral, rat): >2000 mg/kg
  Corrosive; irritating to skin, mucous membranes and eyes

- Recommended:
  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 color, hydrogen chloride, octanoic acid and anhydride.

TRANSPORTATION

Refer to MSDS.

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