

DATA SHEET Nr 1075 F ISONONANOYL CHLORIDE INCL

$\begin{array}{cccc} CH_3 & O \\ | & | \\ CH_3 - C - CH_2 - CH - CH_2 - C \\ | & | & | \\ CH_3 & CH_3 & CI \end{array}$

Molecular formula:	C ₉ H ₁₇ ClO
Molecular weight:	176.7
CAS number:	36727-29-4
EC number:	253-168-4

SYNONYM

3,5,5-trimethylhexanoyl chloride

APPEARANCE

Clear liquid with pungent odor.

PHYSICAL PROPERTIES

Density (20 °C):0.94 g/cm³Boiling point:190 °C/101 kPa

Solubility:

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

CHEMICAL PROPERTIES

- Reacts by hydrolysis yielding hydrochloric acid and isononanoic acid.
- Reacts with amines yielding amides.
- Reacts with alcohols yielding esters.

USES

- Intermediate for organic synthesis.
- Synthesis intermediate for polymerization initiators.



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SPECIFICATION

Parameter	Guaranteed value	Method	Operating procedure
Appearance	Clear liquid	Visual	
Color	\leq 30 APHA	Colorimetry	C – 210
Total C ₉ chlorides	≥98.0 %	Gas chromatography	GC – 421
3,5,5-trimethylhexanoyl chloride	≥ 96.0 %	Gas chromatography	GC - 421
Alpha ramified chlorides	$\leq 2.0 \%$	Gas chromatography	GC – 421
Phosgene	≤ 0.05 %	Iodometry	I – 230
Hydrogen chloride	≤ 0.1 %	Acidimetry	A – 220
Isononanoic acid	≤ 0.1 %	Gas chromatography	GC – 421
Isononanoic anhydride	≤ 1.0 %	Gas chromatography	GC – 421
Carbon tetrachloride	≤ 0.03 %	Gas chromatography	GC - 421
2-Ethylhexanoyl chloride	≤ 0.15 %	Gas chromatography	GC - 421

PACKAGING

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

HANDLING PRECAUTIONS

- <u>Physicochemical hazard:</u> Flash point (closed cup): 79 °C
- <u>Health hazards:</u> LD 50 (oral, rat): 1700 mg/kg LC 50 (inhalation, rat): 0.06-0.1mg/l/1h Irritating on skin, mucous membrane and eyes. Corrosive.
- <u>Recommended:</u>

Avoid contact with alkaline products. Wear gloves, goggles, mask and protective clothes. If eyes are contaminated wash immediately with clean water for at least 15 minutes.

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If concentrated vapors are inhaled carry person into fresh air.

- In both cases call a physician.
- <u>Neutralization:</u> Neutralize by reaction with an alkaline solution.

STORAGE

Stored in its closed original drum in a covered, dry, cool and well-ventilated warehouse the product is stable.

However, 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, isononanoic acid and anhydride levels.

TRANSPORTATION

Refer to MSDS.



