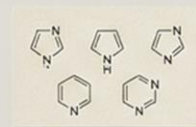




Trichloroacetonitrile



PRODUCT IN FOCUS



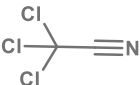
Trichloroacetonitrile

INTRODUCTION

Trichloroacetonitrile is a halogenated organic compound belonging to nitrile family. Its strong electrophilic character makes it a valuable intermediate in organic synthesis. It readily undergoes hydrolysis, particularly under acidic or basic conditions, yielding trichloroacetamide and related derivatives.

MANUFACTURE

Trichloroacetonitrile is typically produced through controlled chlorination of acetonitrile. This involves free radical substitution, where hydrogen atoms on the methyl group are progressively replaced by chlorine. Alternative approach involves dehydration of trichloroacetamide.

Synonyms	Cyanotrichloromethane; 2,2,2-Trichloroacetonitrile; NSC 66405
CAS no.	545-06-2
EINECS no.	208-885-7
Molecular formula	C_2Cl_3N
Molecular weight	144.39
Structure	

APPLICATIONS

Trichloroacetonitrile is a valuable intermediate with a range of applications. Its utility comes from presence of two strong electron withdrawing groups (CCl_3 and CN), which allow diverse chemical transformations.

⊗ Pharmaceutical Intermediates:

- Used in the synthesis of heterocyclic compounds (e.g., imidazoles, triazines, pyrimidines, oxadiazoles, etc).
- Acts as a building block for API intermediates, especially where strong electron-withdrawing groups are required.
- Useful in cyanation reactions to introduce nitrile functionality into drug molecules.

⊗ Agrochemical Applications:

- Serves as an intermediate in the synthesis of Herbicides, Fungicides and Insecticides.
- Enables synthesis of chlorinated nitrile-based bioactive molecules.
- Used in developing crop protection agents due to its reactivity toward nucleophiles.

⊗ Organic Synthesis & Fine Chemicals:

- Functions as a reactive nitrile source in multi-step synthesis.
- Used in C-C and C-N bond formation reactions.
- Acts as a precursor for: amides, carboxylic acids (via hydrolysis), amidines and imidates.

⊗ Heterocyclic Chemistry:

- Acts as a key reagent for preparation of:
- Nitrogen-containing heterocycles.
 - Fused ring systems.
 - Facilitates ring closure reactions due to its activated nitrile group.

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SPECIFICATIONS

Test	Unit	Specification
Appearance	-	Colourless yellow-brown liquid, free from visible impurities
Identification (by IR)	-	Should conform to the structure
Purity (by GC):	-	
Trichloroacetonitrile	%	NLT 98.5
Single Unknown Impurity	%	NMT 0.5
Moisture (by KF)	%	NMT 0.1

STORAGE & PRECAUTION

Keep container tightly closed. Store in well-ventilated area.

PACKING

UN Approved drums;

Packaging quantities (net weight/volume per container): 30 kg/drum, 250 kg/drum

Primary Packaging (material of construction of packaging and closure): Plastic drums

REACH Status

Not registered

ExSyn offers Trichloroacetonitrile on a commercial scale and welcomes your enquiries. Regardless of the quantity required, our commitment to exceptional quality and reliable service makes ExSyn the preferred supplier of choice. Should you require any additional information or the SDS, please feel free to contact us.