

## PRODUCT IN FOCUS



# Trifluoroacetic Acid

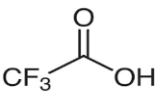
### INTRODUCTION

Trifluoroacetic acid (TFA), is widely used in organic synthesis as a solvent, catalyst and reagent thanks to its reactivity and stability under adverse conditions.

It is considered one of the most economical fluorinated building blocks. It is widely used in peptide synthesis and other organic transformations involving deprotection of t-BOC group.

### Manufacture

Trifluoroacetic acid is commonly produced in Simon electro-fluorination process involving hydrogen fluoride and acetic acid.

<b>Synonyms</b>	Trifluoroethanoic acid Perfluoroacetic acid
<b>CAS no.</b>	76-05-1
<b>EINECS no.</b>	200-929-3
<b>Molecular formula</b>	$C_2HF_3O_2$
<b>Molecular weight</b>	114.02
<b>Structure</b>	

### General Usage

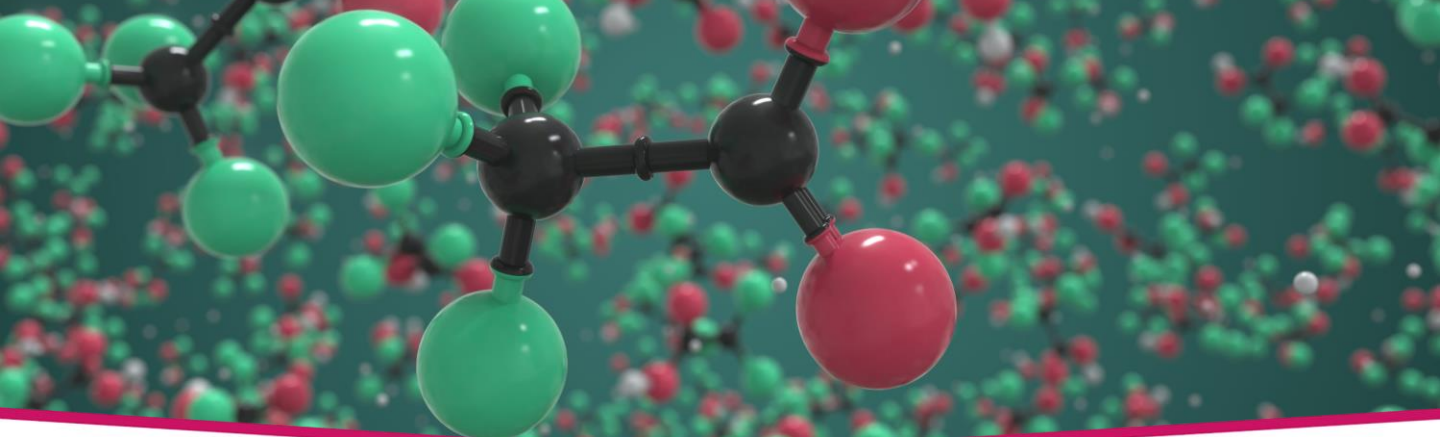
The acid owes its multiple usages to its low boiling point, high dielectric constant, and relatively stronger acidity. It is generally employed in chemical industry as:

- Y Solvent in polymerization and oxidation
- Y Solvent for chromatography
- Y Catalyst in esterification, transesterification, and olefin reduction in petroleum refining
- Y Low Boiling Reagent in various reactions

### Niche' Applications

The chemical processes, that lead to value added products, are centered around the carboxylic group of trifluoroacetic acid and the stability rendered by the trifluoromethyl group. The special applications include:

- Y Trifluoromethylation – introduction of CF<sub>3</sub> group in organic molecules thereby creating CF<sub>3</sub> building blocks
- Y Hydroacylation of complex organic molecules
- Y Acylation of aromatics to form corresponding ketones and a plethora of acyl-containing intermediates
- Y Olefin Hydration to produce alcohols - it replaces sulphuric acid, to which olefins are sensitive
- Y Deprotection of amino group in some peptide synthesis for its higher solvency and volatility
- Y Rearrangement – the acid is a key reagent in converting cyclohexanone oxime to ε-caprolactam
- Y Protein Synthesis – where the acid protects the active amine



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### Proxime Intermediates

The fluorinated acetic acid, by conventional synthetic processes, is easily converted to next step intermediates, that are vital for pharma and agro industries.

In these processes as well, the active carboxylic group and the stable trifluoromethyl moiety are the factors responsible.

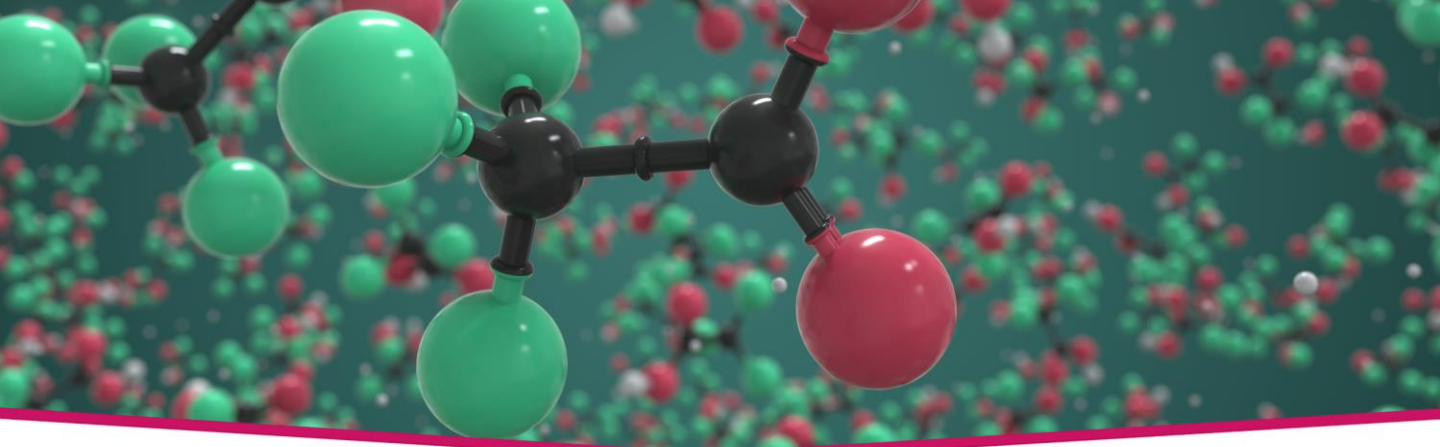
These include:

- Y Trifluoroacetic anhydride – that further produces Thiazafluron
- Y Trifluoroacetic acid ethyl ester (also known as ethyl trifluoroacetate)
- Y Trifluoroacetic acid methyl ester
- Y Trifluoroacetic acid isopropyl ester
- Y 2,2,2-Trifluoroethanol – that is in turn consumed to make isoflurane and polythiazide

### High-End Intermediates

Trifluoroacetic acid finds applications as a key raw material to manufacture number of value-added, high-end intermediates such as:

- Y Peroxytrifluoroacetic acid
- Y 2-(2,2,2-Trifluoroacetylamino)pyridine
- Y N[1-{6-Chloro-3-pyridinyl)methyl}-2(1H)-pyridinylidene]-2,2,2, trifluoroacetamide
- Y Methyl 2-Fluoroacrylate



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### SPECIFICATIONS

Test	Unit	Specification
Appearance	-	Clear & colorless liquid
Moisture	% w/w	0.05 max
Fluoride	% w/w	0.005 max
Chloride	% w/w	0.001 max
Sulphate	% w/w	0.001 max
Arsenic	ppm	NMT 8.0
Titrimetric Purity	% w/w	99.9 min
Identification by Ion Chromatography		The retention time of TFA matches to that of the standard TFA

### REACH status

TFA offered by ExSyn is registered under EU REACH regulations.

### STORAGE

Product is stored at ambient temperature.

ExSyn offers this product on commercial scale and welcomes enquiries. No matter the quantity you need, our exceptional quality and service will make ExSyn your supplier of choice! If you need any additional information or SDS, please get in touch with us.