

Revision 15. Nov. 2024

[Classification by use]

1-1.Medical and agrochemical intermediate raw material

No.	Chemical formula (Classification)	Name	CAS No.	Remarks
1	$F \xrightarrow{CH_3} CH_3$ CF_3COCH_3 (Carbonyl compound)	1,1,1-Trifluoroacetone	421-50-1	Raw material for the therapeutic agent of sickle cell disease and congenital hemolytic anemia.
2	$F \xrightarrow{F} 0 \xrightarrow{CH_3} 0$ $CF_3COCH_2COOC_2H_5$ (Carboxylic acid and derivative)	Ethyl 4,4,4- trifluoroacetoacetate	372-31-6	Pyrazole oxime derivative pesticide raw material. (insecticidal/ rooting)
3	$F \rightarrow F + F + F + F + F + F + F + F + F + $	2,2,2-Trifluoro acetamidine	354-37-0	Cyclooxygenase inhibitory / analgesic trifluoromethyl- triazole derivative raw material.
4	F F O CF ₃ COCH ₂ Br (Carbonyl compound)	3-Bromo-1,1,1- trifluoroacetone	431-35-6	Imidazole pyridine ring skeleton synthetic raw material for non-acidic non- steroidal anti-inflammatory drug.
5	$F \xrightarrow{F} NH_2$ F CF_3CH_2NH_2 (Amine)	2,2,2-Trifluoro ethylamine	753-90-2	Benzodiazepine skeleton modification raw material with trifluoroethyl group.
6	$F \xrightarrow{F} F = 0$ $F \xrightarrow{F} F = 0$ $G_{6}F_{5}-SO_{2}CI$ (Sulfur compound)	Pentafluorobenzene sulfonyl chloride	832-53-1	Sulfur agent raw material with a pentafluorobenzene group, which is highly active in suppressing Zika virus.



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7	$F \rightarrow F = F$ $F \rightarrow F$	Hexafluorobenzene	392-56-3	Pyrimidine amine derivative raw material for wheat red rust diseases.
8	F F F C ₂ F ₅ (CH ₂) ₃ OH (Alcohol)	Pentafluoropentanol	148043-73-6	Fluoroalkyl group side chain component of Fulvestrant, a treatment for breast cancer.
9	$H_{3C} \longrightarrow F_{F}$ (Carbonyl compound)	Trifluoroacetaldehyde methyl hemiacetal (tech.)	431-46-9	A method of introducing a chiral β -CF3 group into a β -amino acid that exhibits a special physiological activity.
10	F F F F F F F F F F F F F F F F F F F	Octafluorotoluene	434-64-0	Selective protection of steroid skeleton enones by perfluorotolyl enol ethers.
11	F F CF ₃ COCH ₂ COCH ₃ (Carbonyl compound)	1,1,1- Trifluoroacetylacetone (abb. TFAcAc)	367-57-7	Synthesis of various derivatives with 2- trifluoromethyl-pyridine skeleton similar to flufenamic acid from TFAcAc.
12	N = - + + + + + + + + + + + + + + + + + +	Trifluoroacetonitrile	353-85-5	Various synthesis examples using TFAN.
13	H ₂ N 4-CF3OC6H4NH2 (Carboxylic acid and derivative)	4-(Trifluoromethoxy) Aniline (abb. TFMA)	461-82-5	Introduced lipophilic -OCF3 group to progranil structure that exhibits strong anticancer activity against bladder cancer and colon cancer cells.

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14	$F = F$ $F = F$ $F = F$ $F_{3}CF_{2}CH_{2}NH_{2}$ $(Amine)$	2,2,3,3,3- Pentafluoropropylamine	422-03-7	Synthesizing a prodrug that binds to the protein-degrading enzyme γ-secretase in cell membranes and confirming its anti- inflammatory effect in kidneys injured by aristolochic acid.
15	F Br Br(CH ₂) ₅ F (Alkane)	1-Bromo-5- fluoropentane	407-97-6	The antiemetic effect of natural cannabinoids (CB) in cancer chemotherapy was recognized, and medical interest in CB (SC) synthesis increased, leading to the discovery of CB receptors. Consideration of SC derivatives with indazole skeleton.
16	F F F CF ₃ CBr=CH ₂ (Alkyne)	2-Bromo-3,3,3- trifluoropropene (abb. BTFB)	1514-82-5	Investigating a new Click reaction synthesis route for Celecoxib, an anti-inflammatory agent with COX-2 inhibitory action, using a novel high-speed continuous flow tube method.
17	F F F CF ₃ CH=CHCN (Carboxylic acid and derivative)	4,4,4- Trifluorocrotononitrile (abb.FMCN)	406-86-0	We have found that C-alkylation of N-alkylindoles and N- alkylpyrroles can proceed in good yields by mixing FMCN and AlBr3 in advance to form a homogeneous catalyst.
18	$F \xrightarrow{F}_{F} F$ $F \xrightarrow{F}_{F} F$ $C5F5N$ (Heterocyclic compound)	Pentafluoropyridine (abb. 5F-Py)	700-16-3	In the synthesis of polypeptides, the protection and deprotection of side chain functional groups are also important factors. We found that the skeleton of 5F-Py is susceptible to nucleophilic attack, and that the phenolic hydroxyl group can be regenerated by a simple deprotection reaction.
19	$F \rightarrow F = F$ $F \rightarrow F$	Pentafluorophenol	771-61-9	In order to simplify the polypeptide synthesis, the amino group of amino acids was protected and the carboxyl group was activated in one step, and good yields of protection and activation were obtained.
20	G F C5Cl2F3N (Benzene derivative)	3,5-Dichloro-2,4,6- trifluoropridine (abb. Cl2F3P)	1737-93-5	In the final process of fluorinated phenoxycarboxylic acid, which has been developed as a plant growth-inhibiting herbicide, the adoption of a reactive distillation apparatus and a change in the catalyst for the ester exchange reaction have resulted in a significant improvement in yield.



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21	F C6H4F2O (Benzene derivative)	2,6-Difluorophenol (abb. 2,6-DFP)	28177-48-2	We investigated a method for synthesizing 4-aminomethyl-2,6- difluorophenol (abb.; ADFP) from 2,6-difluorophenol. Furthermore, we found that the combined use of GABA and ADFP suppressed the binding to GABA receptors by approximately 30% (the first time for a bioisosteric structure of GABA).
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