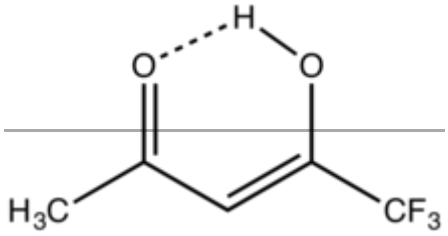
1,1,1-Trifluoroacetylacetone

1,1,1-Trifluoroacetylacetone	
	
Names	
Preferred IUPAC name 1,1,1-Trifluoropentane-2,4-dione	
Other names 1,1,1-Trifluoro-2,4-pentanedione, (trifluoroacetyl)acetone, 1,1,1-(trifluoroacetyl)acetone, 1,1,1-TFAA	
Identifiers	
CAS Number	367-57-7 (https://commonchemistry.cas.org/detail?cas_rn=367-57-7)
3D model (JSmol)	Interactive image (https://chemapps.stolaf.edu/jmol/jmol.php?model=CC%28%3DO%29CC%28%3DO%29C%28F%29%28F%29F)
ChemSpider	66573 (https://www.chemspider.com/Chemical-Structure.66573.html)
ECHA InfoCard	100.006.090 (https://echa.europa.eu/substance-information/-/substanceinfo/100.006.090)
EC Number	206-698-5
PubChem CID	73943 (https://pubchem.ncbi.nlm.nih.gov/compound/73943)
UNII	9N20A8G8SW (https://precision.fda.gov/uniisearch/srs/unii/9N20A8G8SW)
CompTox Dashboard (EPA)	DTXSID3059896 (https://comptox.epa.gov/dashboard/chemical/details/DTXSID3059896)
InChI	
InChI=1S/C5H5F3O2/c1-3(9)2-4(10)5(6,7)8/h2H2,1H3 Key: SHXHPUAKLCCLDV-UHFFFAOYSA-N	
SMILES	
CC(=O)CC(=O)C(F)(F)F	
Properties	
Chemical formula	$C_5H_4F_3O_2$
Molar mass	153.080 g·mol^{-1}
Appearance	colorless liquid
Density	1.27 g/cm^3

Hazards	
GHS labelling:	
Pictograms	
Signal word	**Warning**
Hazard statements	H226, H302, H312, H315, H319, H332
Precautionary statements	P210, P233, P240, P241, P242, P243, P261, P264, P270, P271, P280, P301+P312, P302+P352, P303+P361+P353, P304+P312, P304+P340, P305+P351+P338, P312, P321, P322, P330, P332+P313, P337+P313, P362, P363, P370+P378, P403+P235, P501
Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa). Infobox references	

1,1,1-Trifluoroacetylacetone is the organofluorine compound with the formula $CF_3C(O)CH_2C(O)CH_3$. It is a colorless liquid. Like other 1,3-diketones, it is used as a precursor to heterocycles, e.g. pyrazoles, and metal chelates.[1] It is prepared by condensation of esters of trifluoroacetic acid with acetone.[2]

According to an analysis by proton NMR spectroscopy, the compound exists predominantly (97% at 33 °C, neat) as the enol. For comparison under the same conditions, the percent enol for acetylacetone and hexafluoroacetylacetone are 85 and 100%, respectively.[3]

References

1. Morris, M. L.; Moshier, Ross W.; Sievers, Robert E. (1967). "Tetrakis(1,1,1-trifluoro-2,4-pentanedionato)zirconium(and Hafnium)". *Inorganic Syntheses*. Vol. 9. pp. 50–52. doi:10.1002/9780470132401.ch15 (https://doi.org/10.1002%2F9780470132401.ch15). ISBN 9780470132401.
2. Henne, Albert L.; Newman, Melvin S.; Quill, Laurence L.; Staniforth, Robert A. (1947). "Alkaline condensation of fluorinated esters with esters and ketones". *Journal of the American Chemical Society*. **69** (7): 1819–20. doi:10.1021/ja01199a075 (https://doi.org/10.1021%2Fja01199a075).
3. Jane L. Burdett; Max T. Rogers (1964). "Keto-Enol Tautomerism in β-Dicarbonyls Studied by Nuclear Magnetic Resonance Spectroscopy. I. Proton Chemical Shifts and Equilibrium Constants of Pure Compounds". *J. Am. Chem. Soc*. **86**: 2105–2109. doi:10.1021/ja01065a003 (https://doi.org/10.1021%2Fja01065a003).