



>>Entry Name: 1,1,1,3,3,3-Hexafluoro-2-propanone, 9CI

Synonym(s): Hexafluoroacetone

CAS Registry Number: 684-16-2

Related CAS Registry Numbers(s): 13098-39-0 34202-69-2 109640-39-3

F_3CCOCF_3

Molecular Formula: $\text{C}_3\text{F}_6\text{O}$

Molecular Weight: 166.023

Accurate Mass: 165.985333

Percentage Composition: C 21.70%; F 68.66%; O 9.64%

Use/Importance: Forms a complex with H_2O_2 which functions as a peracid in synthesis. Reagent for gc anal. of amino acids and for the ^{19}F nmr anal. of alcohols and phenols

Physical Description: Gas

Melting Point: Fp -129°

Boiling Point: Bp -26°

pKa Value: $\text{p}K_{\text{a}}$ 6.58 (hydrate)

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 191 mg/kg. LC₅₀ (rat, ihl) 275 ppm (3h exposure). Exp. reprod. and teratogenic effects (by skin absorption)

Aldrich: 29535-3

>>Derivative: Covalent hydrate

Synonym(s): 1,1,1,3,3,3-Hexafluoro-2,2-propanediol

CAS Registry Number: 10543-95-0

Molecular Formula: $\text{C}_3\text{H}_2\text{F}_6\text{O}_2$

Molecular Weight: 184.038

Accurate Mass: 183.995898

Percentage Composition: C 19.58%; H 1.10%; F 61.94%; O 17.39%

Boiling Point: Bp₉₃ 57°

>>Derivative: Semicarbazone

Melting Point: Mp 154°

>>Derivative: Imine

CAS Registry Number: 1645-75-6

Molecular Formula: $\text{C}_3\text{HF}_6\text{N}$

Molecular Weight: 165.038

Accurate Mass: 165.001317

Percentage Composition: C 21.83%; H 0.61%; F 69.07%; N 8.49%

Boiling Point: Bp $15.5-17^\circ$

>>Derivative: Di-Me ketal

Synonym(s): 1,1,1,3,3,3-Hexafluoro-2,2-dimethoxypropane

CAS Registry Number: 754-50-7

Molecular Formula: $\text{C}_5\text{H}_6\text{F}_6\text{O}_2$

Molecular Weight: 212.092

Accurate Mass: 212.027198

Percentage Composition: C 28.32%; H 2.85%; F 53.75%; O 15.09%

Boiling Point: Bp 85°

Refractive Index: n_{D}^{20} 1.3060

Aldrich: 39034-8

References: