>>**Entry Name: 1,1,1,3,3,3-Hexafluoro-2-propanone,** 9Cl
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: C_3F_6O
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: pK_a 6.58 (hydrate)
Hazard & Toxicity: Skin irritant. LD_{50} (rat, orl) 191 mg/kg. LC_{50} (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: $C_3H_2F_6O_2$
Molecular Weight: 184.038
Accurate Mass: 183.995898
Percentage Composition: C 19.58%; H 1.10%; F 61.94%; O 17.39%
Boiling Point: Bp_{93} 57°

>>**Derivative:** Semicarbazone

Melting Point: Mp 154°

>>**Derivative:** Imine

CAS Registry Number: 1645-75-6
Molecular Formula: C_3HF_6N
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°

>>**Derivative:** Di-Me ketal
Synonym(s): 1,1,1,3,3,3-Hexafluoro-2,2-dimethoxypropane

CAS Registry Number: 754-50-7
Molecular Formula: $C_5H_6F_6O_2$
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: