



>>Entry Name: **1,1,1-Trifluoro-2-propanone**, 9CI, 8CI
Synonym(s): 1,1,1-Trifluoroacetone. Acetyltrifluoromethane

CAS Registry Number: 421-50-1
F3CCOCH3

Molecular Formula: C3H3F3O
Molecular Weight: 112.051
Accurate Mass: 112.013599
Percentage Composition: C 32.16%; H 2.70%; F 50.87%; O 14.28%
Use/Importance: Used in aldol condensations
Physical Description: Liq.
Boiling Point: Bp 21.5-22.5°
Other Data: Hygroscopic
Hazard & Toxicity: Lachrymator

Aldrich: T6280-4
Fluka: 91680

>>Derivative: Oxime

CAS Registry Number: 431-40-3
Molecular Formula: C3H4F3NO
Molecular Weight: 127.066
Accurate Mass: 127.024498
Percentage Composition: C 28.36%; H 3.17%; F 44.85%; N 11.02%; O 12.59%
Physical Description: Liq.
Boiling Point: Bp 102-104°
pKa Value: pK_a 6

>>Derivative: Hydrazone

CAS Registry Number: 34226-09-0
Molecular Formula: C3H5F3N2
Molecular Weight: 126.081
Accurate Mass: 126.040482
Percentage Composition: C 28.58%; H 4.00%; F 45.21%; N 22.22%
Physical Description: Liq.
Boiling Point: Bp₂₀ 51-51.5°

>>Variant: enol-form

Molecular Formula: C3H3F3O
Molecular Weight: 112.051
Accurate Mass: 112.013599
Percentage Composition: C 32.16%; H 2.70%; F 50.87%; O 14.28%

>>Derivative: Ac
Synonym(s): 1-(Trifluoromethyl)vinyl acetate

CAS Registry Number: 2247-91-8
Molecular Formula: C5H5F3O2
Molecular Weight: 154.089
Accurate Mass: 154.024164
Percentage Composition: C 38.97%; H 3.27%; F 36.99%; O 20.77%
Boiling Point: Bp 88°
Density: d₂₅²⁵ 1.21
Refractive Index: n_D²⁵ 1.3380

References: