



>>Entry Name: 3,3,3-Trifluoropropanal, 9CI

CAS Registry Number: 460-40-2

F₃CCH₂CHO

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%

Physical Description: Liq.

Boiling Point: Bp₇₄₅ 56-56.5°

Density: d₄²⁰ 1.37

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 150.2-150.8°

>>Variant: enol-form

Synonym(s): 3,3,3-Trifluoro-1-propen-1-ol

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: Me ether

Synonym(s): 3,3,3-Trifluoro-1-methoxy-1-propene

CAS Registry Number: 26885-71-2

Extra CAS Registry Numbers(s): 26885-67-6

Molecular Formula: C₄H₅F₃O

Molecular Weight: 126.078

Accurate Mass: 126.029249

Percentage Composition: C 38.11%; H 4.00%; F 45.21%; O 12.69%

Physical Description: Liq.

Other Data: Predominantly (Z)-form

References:

Henne, A.L. *et al.*, *J.A.C.S.*, 1950, **72**, 3370, (*synth*)

Hong, F. *et al.*, *Chem. Comm.*, 1996, 57-58, (*Me ether, synth, pmr, F-19 nmr*)