



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

CAS Registry Number: 920-66-1

Related CAS Registry Numbers(s): 38701-74-5

$\text{F}_3\text{CCH}(\text{OH})\text{CF}_3$

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

Molecular Weight: 168.039

Accurate Mass: 168.000983

Percentage Composition: C 21.44%; H 1.20%; F 67.84%; O 9.52%

Use/Importance: Chromatographic derivatisation reagent for carboxylic acids; polar solvent

Physical Description: Liq.

Boiling Point: Bp 57-58°

Density: $d_{20.5}$ 1.46

pKa Value: $\text{p}K_{\text{a}1}$ 9.3 (25°)

Hazard & Toxicity: Severe eye irritant. LD_{50} (mus, orl) 600 mg/kg

Aldrich: 32524-4

Fluka: 52512

Sigma: H8508

>>Derivative: Benzoyl

CAS Registry Number: 10315-85-2

Molecular Formula: $\text{C}_{10}\text{H}_6\text{F}_6\text{O}_2$

Molecular Weight: 272.147

Accurate Mass: 272.027198

Percentage Composition: C 44.13%; H 2.22%; F 41.89%; O 11.76%

Physical Description: Cryst. (pentane)

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 67674-48-0

Melting Point: Mp 39-40°

Other: Oakwood 1511

>>Derivative: 2-Methyl-2-propenoyl

References:

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Knunyants, I.L. *et al.*, *CA*, 1962, **57**, 12305i, (rev)

Middleton, W.J. *et al.*, *J.A.C.S.*, 1964, **86**, 4948, (synth)

Urry, W.H. *et al.*, *J.O.C.*, 1967, **32**, 347, (ester)

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