



>>Entry Name: 1,1,1,3,3,3-Hexafluoro-2-phenyl-2-propanol

Synonym(s): α,α -Bis(trifluoromethyl)benzenemethanol, 9CI. α,α -Bis(trifluoromethyl)benzyl alcohol, 8CI

CAS Registry Number: 718-64-9

(F₃C)₂CPhOH

Molecular Formula: C₉H₆F₆O

Molecular Weight: 244.136

Accurate Mass: 244.032283

Percentage Composition: C 44.28%; H 2.48%; F 46.69%; O 6.55%

Boiling Point: Bp 152-155°. Bp₂₄ 95-97°

Density: d 1.45

pKa Value: pK_a 8.8

Refractive Index: n_D³⁰ 1.4133

Aldrich: 10756-5

>>Derivative: Ac

CAS Registry Number: 40999-29-9

Molecular Formula: C₁₁H₈F₆O₂

Molecular Weight: 286.173

Accurate Mass: 286.042848

Percentage Composition: C 46.17%; H 2.82%; F 39.83%; O 11.18%

Melting Point: Mp 45-47°

>>Derivative: Benzoyl

CAS Registry Number: 40999-26-6

Molecular Formula: C₁₆H₁₀F₆O₂

Molecular Weight: 348.244

Accurate Mass: 348.058498

Percentage Composition: C 55.18%; H 2.89%; F 32.73%; O 9.19%

Melting Point: Mp 47.5-49°

>>Derivative: 4-Nitrobenzoyl

CAS Registry Number: 57633-49-5

Melting Point: Mp 138-139°

>>Derivative: 4-Chlorobenzoyl

Melting Point: Mp 90-91°

References:

- Knunyants, I.L. *et al.*, *Izv. Akad. Nauk SSSR, Otd. Khim. Nauk*, 1960, 686; *CA*, **54**, 22485a, (*synth*)
Olah, G.A. *et al.*, *J.A.C.S.*, 1966, **8**, 3310-3312, (*pmr*, *F-19 nmr*)
Brownlee, R.T.C. *et al.*, *J.A.C.S.*, 1968, **90**, 1757-1767, (*synth*, *ir*)
Chang, I.S. *et al.*, *Can. J. Chem.*, 1972, **50**, 512-520, (*synth*, *props*)
Martin, J.C. *et al.*, *J.A.C.S.*, 1975, **97**, 6137, (*derivs*, *synth*, *pmr*, *F-19 nmr*)