



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

Synonym(s): Perfluoro-*tert*-butanol

CAS Registry Number: 2378-02-1

Related CAS Registry Numbers(s): 17526-77-1 29646-16-0

(F₃C)₃COH

Molecular Formula: C₄HF₉O

Molecular Weight: 236.037

Accurate Mass: 235.988367

Percentage Composition: C 20.35%; H 0.43%; F 72.44%; O 6.78%

Use/Importance: Source of (F₃C)₃CO⁽⁻⁾ ions

Physical Description: Liq.

Boiling Point: Bp 44-45°

pKa Value: pK_a 5.2 (25°)

Other Data: Forms Na and K salts

Aldrich: 33102-3

Fluka: 77257

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 280C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 260C, (*ir*)

Filler, R. *et al.*, *J.O.C.*, 1967, **32**, 1217, (*synth*)

Yokozeki, A. *et al.*, *J. Phys. Chem.*, 1975, **79**, 155, (*ed*)