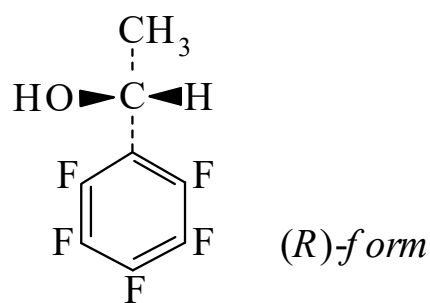




>>Entry Name: 1-(Pentafluorophenyl)ethanol

Synonym(s): 2,3,4,5,6-Pentafluoro- α -methylbenzenemethanol, 9CI. 2,3,4,5,6-Pentafluoro- α -methylbenzyl alcohol, 8CI



CAS Registry Number: 830-50-2

Molecular Formula: $C_8H_5F_5O$

Molecular Weight: 212.119

Accurate Mass: 212.026055

Percentage Composition: C 45.30%; H 2.38%; F 44.78%; O 7.54%

>>Variant: (R)-form

CAS Registry Number: 104371-21-3

Molecular Formula: $C_8H_5F_5O$

Molecular Weight: 212.119

Accurate Mass: 212.026055

Percentage Composition: C 45.30%; H 2.38%; F 44.78%; O 7.54%

Physical Description: Cryst. (pentane)

Melting Point: Mp 42.5-43°

Optical Rotation: $[\alpha]_D^{29} +7$ (c, 1.1 in pentane)

Aldrich: 42187-1

Fluka: 76744

>>Variant: (S)-form

CAS Registry Number: 104371-20-2

Molecular Formula: $C_8H_5F_5O$

Molecular Weight: 212.119

Accurate Mass: 212.026055

Percentage Composition: C 45.30%; H 2.38%; F 44.78%; O 7.54%

Physical Description: Cryst. (pentane or by subl.)

Melting Point: Mp 42°

Optical Rotation: $[\alpha]_D^{28} -7.1$ (c, 1.0 in pentane)

Aldrich: 42189-8

Fluka: 76746

>>Variant: ($\pm$)-form

CAS Registry Number: 75853-08-6

Molecular Formula: $C_8H_5F_5O$

Molecular Weight: 212.119

Accurate Mass: 212.026055

Percentage Composition: C 45.30%; H 2.38%; F 44.78%; O 7.54%

Boiling Point: Bp₃₀ 102-103°

Refractive Index: n_D^{17} 1.4394

Aldrich: 23293-9

Fluka: 76748

References:

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