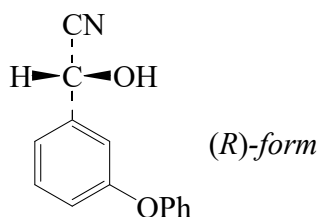




>>Entry Name: α -Hydroxy-3-phenoxybenzeneacetonitrile, 9CI

Synonym(s): α -Cyano-3-phenoxybenzyl alcohol



CAS Registry Number: 39515-47-4

Extra CAS Registry Numbers(s): 52315-06-7

Molecular Formula: $C_{14}H_{11}NO_2$

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Use/Importance: Starting material for pyrethroid insecticides, e.g. Cypermethrin [DKZ00-R](#)

>>Variant: (*R*)-form

CAS Registry Number: 71962-66-8

Molecular Formula: $C_{14}H_{11}NO_2$

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{+16}$ (c, 1.0 in C_6H_6)

>>Derivative: Ac

CAS Registry Number: 126641-87-0

Molecular Formula: $C_{16}H_{13}NO_3$

Molecular Weight: 267.284

Accurate Mass: 267.089544

Percentage Composition: C 71.90%; H 4.90%; N 5.24%; O 17.96%

Optical Rotation: $[\alpha]_D^{25}-7.02$ (c, 1 in $CHCl_3$)

>>Variant: (*S*)-form

CAS Registry Number: 61826-76-4

Molecular Formula: $C_{14}H_{11}NO_2$

Molecular Weight: 225.246

Accurate Mass: 225.078979

Percentage Composition: C 74.65%; H 4.92%; N 6.22%; O 14.21%

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{20}-29.4$ (c, 0.4 in $CHCl_3$)

>>Derivative: Ac

CAS Registry Number: 113301-28-3

Molecular Formula: $C_{16}H_{13}NO_3$

Molecular Weight: 267.284

Accurate Mass: 267.089544

Percentage Composition: C 71.90%; H 4.90%; N 5.24%; O 17.96%

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{27}+21.25$ (c, 10.27 in C_6H_6)

References:

Martel, J.J. *et al.*, *Pestic. Sci.*, 1980, **11**, 188-201, (*resoln*)

Anderson, R.J. *et al.*, *J. Agric. Food Chem.*, 1985, **33**, 508-514, (*synth*)

Inagaki, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 111-120, (*Ac*)

Brown, R.F.C. *et al.*, *Tetrahedron*, 1994, **50**, 13739-13752, (*R*-form, *synth*, *ir*, *pmr*, *ms*)

Fishman, A. *et al.*, *Tetrahedron: Asymmetry*, 1998, **9**, 107-118, (*S*-form, *synth*, *pmr*, *ms*)