



>>Entry Name: 1-(4-Nitrophenyl)ethanol

Synonym(s): α -Methyl-4-nitrobenzenemethanol, 9Cl. α -Methyl-*p*-nitrobenzyl alcohol, 8Cl. Methyl *p*-nitrophenylcarbinol. α -Hydroxyethyl-*p*-nitrobenzene

CAS Registry Number: 6531-13-1

Related CAS Registry Numbers(s): 73104-87-7

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

>>Variant: (*S*)-form

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Optical Rotation: $[\alpha]_{\text{D}}^{20} -27.3$ (c, 2.42 in CHCl₃)

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

CAS Registry Number: 99531-06-3

Molecular Formula: C₈H₉NO₃

Molecular Weight: 167.164

Accurate Mass: 167.058244

Percentage Composition: C 57.48%; H 5.43%; N 8.38%; O 28.71%

Physical Description: Sweet-tasting viscous yellow oil

Boiling Point: Bp₁₆ 158°. Bp₂ 137-138°

>>Derivative: Ac

CAS Registry Number: 19759-27-4

Molecular Formula: C₁₀H₁₁NO₄

Molecular Weight: 209.201

Accurate Mass: 209.068809

Percentage Composition: C 57.41%; H 5.30%; N 6.70%; O 30.59%

Physical Description: Prisms (petrol)

Melting Point: Mp 55-56°

Boiling Point: Bp₁₆ 161-163°

>>Derivative: 4-Nitrobenzoyl

CAS Registry Number: 54059-80-2

Melting Point: Mp 138-138.4°

References:

v. Braun, J. *et al.*, *Ber.*, 1913, **46**, 3050-3055, (*synth*)

Ford-Moore, H.A. *et al.*, *J.C.S.*, 1946, 679-681, (*Ac*)

Fuchs, R. *et al.*, *J.A.C.S.*, 1954, **76**, 1631-1634, (*synth*)

Nezhuta, E.I. *et al.*, *Zh. Obshch. Khim.*, 1957, **27**, 1079-1080; *J. Gen. Chem. USSR (Engl. Transl.)*, 1957, **27**, 1163-1164, (*synth*)

Cabaret, D. *et al.*, *Tet. Lett.*, 1984, **25**, 547, (*synth, abs config*)

Akakabe, Y. *et al.*, *J.C.S. Perkin I*, 1995, 1295, (*S-form*)