



>>Entry Name: (4-Hydroxyphenoxy)acetic acid, 9CI

CAS Registry Number: 1878-84-8

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Physical Description: Needles (toluene)

Melting Point: Mp 152°

Aldrich: 43939-8

>>Derivative: Anilide

CAS Registry Number: 29813-84-1

Molecular Formula: C₁₄H₁₃NO₃

Molecular Weight: 243.262

Accurate Mass: 243.089544

Percentage Composition: C 69.12%; H 5.39%; N 5.76%; O 19.73%

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 101°

>>Derivative: Me ether

Synonym(s): (4-Methoxyphenoxy)acetic acid, 9CI

CAS Registry Number: 1877-75-4

Molecular Formula: C₉H₁₀O₄

Molecular Weight: 182.176

Accurate Mass: 182.05791

Percentage Composition: C 59.34%; H 5.53%; O 35.13%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 108-110°

Rare Chemicals Library: S61665-6

>>Derivative: Me ether, Et ester

CAS Registry Number: 18598-23-7

Molecular Formula: C₁₁H₁₄O₄

Molecular Weight: 210.229

Accurate Mass: 210.08921

Percentage Composition: C 62.85%; H 6.71%; O 30.44%

Physical Description: Oil

Boiling Point: Bp_{0.01} 102-105°

>>Derivative: Trifluoromethyl ether

CAS Registry Number: 72220-50-9

Molecular Formula: C₉H₇F₃O₄

Molecular Weight: 236.147

Accurate Mass: 236.029644

Percentage Composition: C 45.78%; H 2.99%; F 24.14%; O 27.10%

Melting Point: Mp 84-86°

References:

Carter, W. *et al.*, *J.C.S.*, 1900, 1222-1227, (*synth, anilide*)

Koelsch, C.F., *J.A.C.S.*, 1931, **53**, 304-305, (*Me ether*)

Bogatskii, A.V., *CA*, 1979, **92**, 22214z, (*trifluoromethyl ether*)

Sankararaman, S. *et al.*, *J.A.C.S.*, 1987, **109**, 5235-5249, (*Me ether, synth, ir, pmr, cmr, ms*)