



Optical Rotation: $[\alpha]_{\text{D}}^{25} +105$ (c, 0.62 in CHCl_3)

>>Derivative: Nitrile

Molecular Formula: $\text{C}_{17}\text{H}_{12}\text{N}_2\text{O}_2$

Molecular Weight: 276.294

Accurate Mass: 276.089878

Percentage Composition: C 73.90%; H 4.38%; N 10.14%; O 11.58%

Physical Description: Cryst. (C_6H_6 /hexane)

Melting Point: Mp 149-152°

Optical Rotation: $[\alpha]_{\text{D}}^{27} -103$ (c, 2 in CHCl_3)

>>Variant: (S)-form

CAS Registry Number: 5123-55-7

Molecular Formula: $\text{C}_{17}\text{H}_{13}\text{NO}_4$

Molecular Weight: 295.294

Accurate Mass: 295.084459

Percentage Composition: C 69.15%; H 4.44%; N 4.74%; O 21.67%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 183-185°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -212$ (c, 2 in EtOH)

Fluka: 79950

Sigma: P4753

>>Derivative: Me ester

CAS Registry Number: 14380-85-9

Molecular Formula: $\text{C}_{18}\text{H}_{15}\text{NO}_4$

Molecular Weight: 309.321

Accurate Mass: 309.100109

Percentage Composition: C 69.89%; H 4.89%; N 4.53%; O 20.69%

Physical Description: Cryst. (C_6H_6 /petrol)

Melting Point: Mp 113-114°

>>Derivative: Et ester

CAS Registry Number: 50468-37-6

Molecular Formula: $\text{C}_{19}\text{H}_{17}\text{NO}_4$

Molecular Weight: 323.348

Percentage Composition: C 70.58%; H 5.30%; N 4.33%; O 19.79%

Physical Description: Cryst. (C_6H_6)

Melting Point: Mp 56-57°

Optical Rotation: $[\alpha]_{\text{D}} -206.2$ (c, 0.5 in C_6H_6)

>>Derivative: Ph ester

CAS Registry Number: 63203-49-6

Molecular Formula: $\text{C}_{23}\text{H}_{17}\text{NO}_4$

Molecular Weight: 371.392

Percentage Composition: C 74.38%; H 4.61%; N 3.77%; O 17.23%

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 130-131°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -158$ (c, 3 in DMF)

>>Derivative: Chloride

CAS Registry Number: 32150-91-7

Molecular Formula: $\text{C}_{17}\text{H}_{12}\text{ClNO}_3$

Molecular Weight: 313.739

Percentage Composition: C 65.08%; H 3.86%; Cl 11.30%; N 4.46%; O 15.30%

Physical Description: Needles (C_6H_6 /petrol)

Melting Point: Mp 84-85°

Optical Rotation: $[\alpha]_{\text{D}}^{21} -235$ (c, 0.4 in C_6H_6)