



>>Entry Name: 4,4'-Ethynediylbisbenzoic acid, 9CI

Synonym(s): 4,4'-Tolandicarboxylic acid

CAS Registry Number: 16819-43-5

Structure by analogy with 2,2'-Ethynediylbisbenzoic acid, [NVF97-I](#)

Molecular Formula: $C_{16}H_{10}O_4$

Molecular Weight: 266.253

Accurate Mass: 266.05791

Percentage Composition: C 72.18%; H 3.79%; O 24.04%

Melting Point: Mp 398-402°

>>Derivative: Di-Me ester

CAS Registry Number: 16882-08-9

Molecular Formula: $C_{18}H_{14}O_4$

Molecular Weight: 294.306

Accurate Mass: 294.08921

Percentage Composition: C 73.46%; H 4.79%; O 21.75%

Physical Description: Cryst.

Melting Point: Mp 226-227°

>>Derivative: Di-Et ester

CAS Registry Number: 83536-13-4

Molecular Formula: $C_{20}H_{18}O_4$

Molecular Weight: 322.36

Accurate Mass: 322.12051

Percentage Composition: C 74.52%; H 5.63%; O 19.85%

Physical Description: Cryst.

Melting Point: Mp 148-149°

>>Derivative: Dichloride

CAS Registry Number: 16819-44-6

Molecular Formula: $C_{16}H_8Cl_2O_2$

Molecular Weight: 303.143

Accurate Mass: 301.990134

Percentage Composition: C 63.39%; H 2.66%; Cl 23.39%; O 10.56%

Physical Description: Cryst. ($CHCl_3$ /hexane)

Melting Point: Mp 143-146°

>>Derivative: Dinitrile

CAS Registry Number: 5216-36-4

Molecular Formula: $C_{16}H_8N_2$

Molecular Weight: 228.253

Accurate Mass: 228.068748

Percentage Composition: C 84.19%; H 3.53%; N 12.27%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 249-252°

References:

Weis, C.D., *Helv. Chim. Acta*, 1965, **49**, 234, (*nitrile, synth*)

Broser, W. *et al.*, *Tet. Lett.*, 1967, 3117, (*synth, ir*)

Lee, B.H. *et al.*, *J. Polym. Sci., Polym. Chem. Ed.*, 1982, **20**, 393, (*synth, ir*)

Nishihara, Y. *et al.*, *J.O.C.*, 2000, **65**, 1780-1787, (*nitrile*)