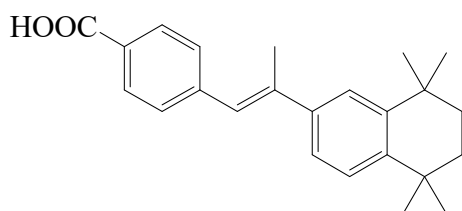




>>Entry Name: 4-[2-(5,6,7,8-Tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]benzoic acid, 9CI

Synonym(s): TTNPB



CAS Registry Number: 101204-37-9

Molecular Formula: C₂₄H₂₈O₂

Molecular Weight: 348.484

Accurate Mass: 348.20893

Percentage Composition: C 82.72%; H 8.10%; O 9.18%

Use/Importance: Retinoic acid receptor antagonist. Shows anticancer activity.

>>Variant: (*E*)-form

CAS Registry Number: 71441-28-6

Molecular Formula: C₂₄H₂₈O₂

Molecular Weight: 348.484

Accurate Mass: 348.20893

Percentage Composition: C 82.72%; H 8.10%; O 9.18%

Physical Description: Solid (CH₂Cl₂/hexane)

Melting Point: Mp 247-248°

>>Derivative: Et ester

CAS Registry Number: 71441-09-3

Molecular Formula: C₂₆H₃₂O₂

Molecular Weight: 376.538

Accurate Mass: 376.24023

Percentage Composition: C 82.94%; H 8.57%; O 8.50%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 96-97°

>>Derivative: Nitrile

CAS Registry Number: 87756-44-3

Molecular Formula: C₂₄H₂₇N

Molecular Weight: 329.484

Accurate Mass: 329.214349

Percentage Composition: C 87.49%; H 8.26%; N 4.25%

Melting Point: Mp 172-173°

References:

Loeliger, P. *et al.*, *Eur. J. Med. Chem. (Chim. Ther.)*, 1980, **15**, 9-15, (*synth*)

U.S. Pat., 1982, 4 326 055; *CA*, **97**, 23436p, (*synth*)

Ger. Pat., 1983, 3 202 125; *CA*, **99**, 194642y, (*nitrile*)

Dawson, M.I. *et al.*, *J.O.C.*, 1984, **49**, 5265-5267, (*Et ester*)