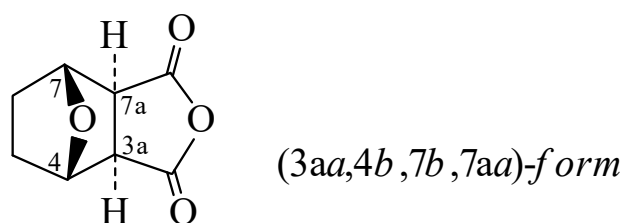




>>Entry Name: Hexahydro-4,7-epoxyisobenzofuran-1,3-dione, 9CI

Synonym(s): Norcantharidin. 7-Oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid anhydride, 8CI



CAS Registry Number: 5442-12-6

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

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

Hazard & Toxicity: LD₅₀ (mus, ivn) 10 mg/kg

Rare Chemicals Library: S31758-6

>>Variant: (3α,4α,7α,7α)-form

Synonym(s): *endo*-form

CAS Registry Number: 51154-98-4

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

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

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 169-170° (158-159°)

Solubility: Insol. Et₂O

>>Variant: (3α,4β,7β,7α)-form

Synonym(s): *exo*-form

CAS Registry Number: 29745-04-8

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

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

Use/Importance: Blocks the root growth of certain plants. Has little or none of the reputed aphrodisiac action

Physical Description: Cryst. or prisms (Me₂CO or Me₂CO/C₆H₆ or by subl.)

Melting Point: Mp 115-117°

References:

Diels, O. *et al.*, *J. Prakt. Chem.*, 1940, **156**, 285, (*synth*)

Winston, A. *et al.*, *J.O.C.*, 1967, **32**, 2166, (*synth*)

Eggelte, T.A. *et al.*, *Tetrahedron*, 1973, **29**, 2445, (*synth*, *pmr*, *ir*)

Ragab, Y.A. *et al.*, *J. Polym. Sci., Polym. Lett. Ed.*, 1976, **14**, 273, (*synth*)

Eggelte, T.A. *et al.*, *J.C.S. Perkin I*, 1978, 980, (*synth*, *ir*)

Csende, F. *et al.*, *Org. Prep. Proced. Int.*, 1999, **31**, 220-222, (*exo-form*, *synth*)