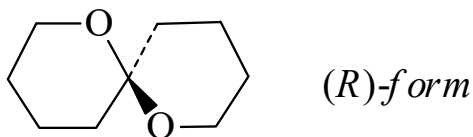




>>Entry Name: 1,7-Dioxaspiro[5.5]undecane, 9CI

Synonym(s): Olean



CAS Registry Number: 180-84-7

Type of Compound Code(s): VA3350 VF8000

Molecular Formula: C₉H₁₆O₂

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Biological Source: Major component of the sex pheromone of the olive fly, *Dacus oleae*

Aldrich: 30130-2

Sigma: D7151

>>Variant: (R)-form

CAS Registry Number: 90839-16-0

Molecular Formula: C₉H₁₆O₂

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{21} -121.6$ (c, 0.1 in pentane)

>>Variant: (S)-form

CAS Registry Number: 90839-15-9

Molecular Formula: C₉H₁₆O₂

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{23} +109.3$ (c, 0.28 in pentane)

>>Variant: (±)-form

Molecular Formula: C₉H₁₆O₂

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Physical Description: Liq.

Boiling Point: Bp₁₃ 77-78°

Other Data: The nat. prod. is racemic; the (R) enantiomer shows greater activity toward male flies and the (S) towards females

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 407B, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 329C, (ir)

Stetter, H. *et al.*, *Chem. Ber.*, 1958, **91**, 2543, (synth)

Micovic, V.M. *et al.*, *Tetrahedron*, 1969, **25**, 985, (synth)

Baker, R. *et al.*, *Chem. Comm.*, 1980, 52, (isol, synth)

Kocienski, P. *et al.*, *Tet. Lett.*, 1983, **24**, 3905, (synth)

Kay, I.T. *et al.*, *Tet. Lett.*, 1983, **24**, 5915, (synth)

Redlich, H. *et al.*, *Angew. Chem., Int. Ed.*, 1984, **23**, 519, (synth)

Ley, S.V. *et al.*, *Tet. Lett.*, 1984, **25**, 113, (synth)

Baker, R. *et al.*, *J.C.S. Perkin I*, 1987, 1123, (isol, synth)

Iwata, C. *et al.*, *Chem. Pharm. Bull.*, 1988, **36**, 3257, (synth)

Marko, I.E. *et al.*, *Tet. Lett.*, 1992, **33**, 1799, (synth)

Yannakopoulou, K. *et al.*, *Angew. Chem., Int. Ed.*, 1996, **35**, 2480-2482, (resoln)

Hayes, P. *et al.*, *Synthesis*, 1999, 783-786, (synth, ir, pmr, cmr, ms)

Uchiyama, M. *et al.*, *Tet. Lett.*, 2001, **42**, 1931-1934, (synth)