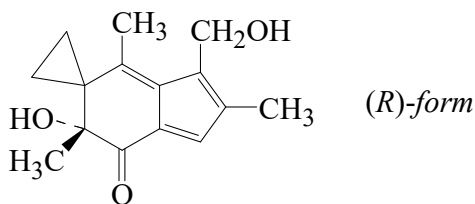




>>Entry Name: Irofulven, INN

Synonym(s): 6'-Hydroxy-3'-(hydroxymethyl)-2',4',6'-trimethylspiro[cyclopropane-1,5'-[5*H*]inden]-7'(6*H*)-one, 9Cl. HMAF. MGI-114



CAS Registry Number: 187277-46-9

Molecular Formula: C₁₅H₁₈O₃

Molecular Weight: 246.305

Accurate Mass: 246.125595

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Biological Use/Importance: Antineoplastic agent

Development Status: Phase I clinical trials

Other Data: Deriv. of 1,7,12-Trihydroxy-2,9-illudadien-8-one [KCL66-S](#)

Other: MGI Pharma

>>Variant: (R)-form

CAS Registry Number: 158440-71-2

Molecular Formula: C₁₅H₁₈O₃

Molecular Weight: 246.305

Accurate Mass: 246.125595

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Physical Description: Yellow cryst.

Melting Point: Mp 127-129°

Optical Rotation: $[\alpha]_D^{25} -639$ (c, 0.1 in EtOH)

References:

- Pat. Coop. Treaty (WIPO)*, 1994, 94 18 151; *CA*, **121**, 230392a, (*synth, pharmacol*)
Kelner, M.J. *et al.*, *Invest. New Drugs*, 1996, **14**, 161-167, (*pharmacol*)
McMorris, T.C. *et al.*, *J. Nat. Prod.*, 1996, **59**, 896-899, (*synth, pmr, cmr, ir, uv, ms*)
Macdonald, J.R. *et al.*, *Cancer Res.*, 1997, **57**, 279-283, (*pharmacol*)
McMorris, T.C. *et al.*, *Chem. Comm.*, 1997, 315-316, (*synth*)