



Formula: C18H16O3

MW: 280.32

CAS: 35212-22-7

MDL: MFCD00221719

TNP:

IPRIFLAVONE; 7-ISOPROPYLOXYISOFLAVONE; 7-Isoproxyisoflavone;
7-ISOPROPOXY-3-PHENYL-4H-1-BENZOPYRAN-4-ONE; 7-ISOPROPOXYISOFLAVONE;
7-(1-methylethoxy)-3-phenyl-4h-1-benzopyron-4-one; YAMBOLAP;
7-(1-methylethoxy)-3-phenyl-4h-1-benzopyran-4-on



LogP: 2.41

LogS: -3.78

Acceptors: 3

Donors: 0

Rotation Bonds: 2

Chiral Centers: 0

N+O: 3

LIPINSKY: 4

IUPAC: 7-(methylethoxy)-3-phenylchromen-4-one

Smiles: c12c(occ(c1=O)c1ccccc1)cc(cc2)OC(C)C

Specification: FINE Chemical & INTERMEDIATES; Iso-Flavones; APIs; Biochemistry;

Flavonoids; Nutraceuticals; Food & Flavor Additives Ipriflavone Chemical Properties:

mp 116-120 C(lit.) Merck 5074 CAS DataBase Reference35212-22-7(CAS DataBase Reference) Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 24/25-36/37/39-27-26 WGK Germany 2 RTECS DJ3100500 Ipriflavone English Ipriflavone Usage And Synthesis Chemical Properties:

white powder Ipriflavone Raw materialsDiethyl ether-->Acetic acid glacial-->Potassium carbonate-->Zinc chloride-->Resorcine-->Benzeneacetonitrile-->Phenylacetic acid-->2-Bromopropane

Merck 13 Reference: Monograph Number: 0005093

Title: Ipriflavone

CAS Registry Number: 35212-22-7

CAS Name: 7-(1-Methylethoxy)-3-phenyl-4H-1-benzopyran-4-one

Additional Names: 7-isopropoxy-3-phenyl-4H-1-benzopyran-4-one;
7-isopropoxy-3-phenylchromone; 7-isopropoxyisoflavone

Manufacturers' Codes: FL-113; TC-80

Trademarks: Iprosten (Takeda); Osten (Takeda); Osteofix (Chiesi); Yambolap (Chinoin)

Molecular Formula: C₁₈H₁₆O₃

Molecular Weight: 280.32.

Percent Composition: C 77.12%, H 5.75%, O 17.12%

Literature References: Isoflavone derivative with anti-anginal and anti-osteopenic activity. Prepn: L. Feuer et al., DE 2125245 (1971 to Chinoin), C.A. 76, 72407e (1972). Use as anabolic in animals: eidem, US 3833730; in humans; eidem, US 3949085 (1974, 1976 both to Chinoin). Cardiovascular properties in stable angina: V. Grubich et al., Lancet 1, 211 (1979). Cardiological effects in animals: L. Feuer et al., Arzneim.-Forsch. 31, 953 (1981). Metabolism and disposition in rats: K. Yoshida et al., Radioisotopes 34, 612, 618 (1985). Effect in rats on estrogen-stimulated calcitonin secretion: I. Yamazaki, Life Sci. 38, 757 (1986); I. Yamazaki, M. Kinoshita, ibid. 1535; on glucocorticoid-induced osteoporosis: I. Yamazaki et al., ibid. 951.

Properties: Crystals from acetone, mp 115-117.

Melting point: mp 115-117

Therap-Cat: Calcium regulator.