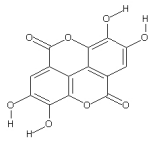

Formula: C14H6O8

MW: 302.2

Salt: H2O

CAS: 476-66-4

TNP NUMBER: TNP00132

MDL NUMBER: MFCD00006914

Smiles: c12c3c4oc(c2cc(O)c(c1oc(c3cc(O)c4O)=O)O)=O

THERAPEUTIC CATEGORY: Hemostatic

REFERENCE: Cited Reference 1. M. Das et al. Biochem. Biophys. Res. Commun. 120, 427, (1984) 2. C. Kluft et al. Adv. Exp. Med. Biol. 156A, 201, (1983) 3. Exner, T. and Rickard, K.A. Thromb. Res. 26, 83, (1982) Reference Majid, S., et al., Influence of ellagic acid on antioxidant defense system and lipid peroxidation in mice. Biochem. Pharmacol. 42, 1441-1445, (1991) abstract Weinder-Wells, M.A., et al., DNA gyrase inhibitory activity of ellagic acid derivatives. Bioorg. Med. Chem. Lett. 8, 97-100, (1998) abstract Constantinou, A., et al., The dietary anticancer agent ellagic acid is a potent inhibitor of DNA topoisomerases in vitro. Nutr. Cancer 23, 121-130, (1995) abstract Gali, H.U., et al., Hydrolyzable tannins: potent inhibitors of hydroperoxide production and tumor promotion in mouse skin treated with 12-O-tetradecanoylphorbol 13-acetate in vivo. Int. J. Cancer 51, 425-432, (1992) abstract Cozzi, R., et al., Taurine and ellagic acid: two differently-acting natural antioxidants. Environ. Mol. Mutagen. 26, 248-254, (1995) abstract Castonguay, A., et al., Biodistribution of, antimutagenic efficacies in Salmonella typhimurium of, and inhibition of P450 activities by ellagic acid and one analogue. Chem. Res. Toxicol. 11, 1258-1264, (1998) abstract Hayatsu, H., et al., Dietary inhibitors of mutagenesis and carcinogenesis. Mutat. Res. 202,

429-446, (1988) abstract Merck Merck 13,3580 Beilstein Beil. 19,V,7,108

SOURCE: A naturally ocurring plant phenol. From tree bark. From kino of Eucaliptus maculata Hook and E. hemifolia

ACCEPTORS: 8

DONORS: 4

ROTATION BONDS: 4

N+O: 8

Chiral Centers: 0

LogP: 1.14

LogS: -3.01

LIPINSKI: 4