



Formula: C₂₀H₂₇NO₁₁

MW: 457.43

CAS: 29883-15-6

MDL: MFCD00066659

TNP: TNP00471

(r)-alpha-((6-o-beta-d-glucopyranosyl-beta-d-glucopyranosyl)oxy)benzeneaceto;
(r)-alpha-((6-o-beta-d-glucopyranosyl-beta-d-glucopyranosyl)oxy)benzeneacetone; (r)-oxy);
(r)-y); amygdalose; benzeneacetonitrile, alpha-((6-o-beta-d-glucopyranosyl-beta-d-glucopyr



LogP: -5.59

LogS: -1.85

Acceptors: 11

Donors: 7

Rotation Bonds: 13

Chiral Centers: 11

N+O: 12

LIPINSKY: 2

IUPAC: 2-phenyl-2-(3,4,5-trihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)(2H-3,4,5,6-tetrahydropyran-2-yloxy)]methyl])(2H-3,4,5,6-tetrahydropyran-2-yloxy))ethanenitrile

Smiles: O1C(C(C(C(O)C1COC1C(C(C(O)C(O1)CO)O)O)O)OC(C#N)c1ccccc1

Physiol Action: Cyanogenic glycoside that is a component of bitter almonds and apricot pits.

There is no scientific evidence that amygdalin itself is an effective anti-cancer agent. Recent studies using β -glucoside linked to a tumor-associated monoclonal antibody to ele

REFERENCE: Syrigos, K.N., et al., In vitro cytotoxicity following specific activation of amygdalin by β -glucosidase conjugated to a bladder cancer-associated monoclonal antibody. *Int. J. Cancer* 78, 712-719, (1998) Moertel, C.G., et al., A clinical trial of amygdalin (Laetrile) in the treatment of human cancer. *New Engl. J. Med.* 306, 201-206, (1982) Chitnis, M.P., et al. , Studies on high-dose chemotherapy of amygdalin in murine P388 lymphocytic leukaemia and P815 mast cell leukaemia. *J. Cancer Res. Clin. Oncol.* 109, 208-209, (1985) Merck Merck 13,601 Beilstein Beil. 17,V,8,118

SOURCE: From apricot kernels. Cynogenic glycoside which occurs in seeds of Rosaceae; principally in bitter almonds; also in peaches and apricots.

ACTIVITY: Cyanogenic glycoside that is a component of bitter almonds and apricot pits. There is no scientific evidence that amygdalin itself is an effective anti-cancer agent. Recent studies using β -glucoside linked to a tumor-associated monoclonal antibody to release cyanide at the tumor cell has shown significant cytotoxicity.

Specification: Miscellaneous Natural Products; Biochemistry; Disaccharides; Glycosides; Sugars; Natural Plant Extract; Nutritional Ingredients Amygdalin Chemical Properties:

mp 223-226 C(lit.) α -38.5