



Formula: C₈H₈O₃

MW: 152.15

CAS: 121-33-5

TNP NUMBER: TNP00461

MDL NUMBER: MFCD00006942

IUPAC: 4-hydroxy-3-methoxybenzaldehyde

Smiles: c1(ccc(cc1OC)C=O)O

Occurs naturally in wide variety of foods and plants. Isolated from vanilla beans

ACCEPTORS: 3

DONORS: 1

ROTATION BONDS: 3

N+O: 3

Chiral Centers: 0

LogP: 1.28

LogS: -2.92

LIPINSKI: 4

Monograph Number: 0009998

Title: Vanillin

CAS Registry Number: 121-33-5

CAS Name: 4-Hydroxy-3-methoxybenzaldehyde

Additional Names: methylprotocatechuic aldehyde; vanillic aldehyde

Trademarks: Rhonavil Extra Pure (Rh