



Formula: C<sub>17</sub>H<sub>18</sub>N<sub>2</sub>O<sub>6</sub>

MW: 346.34

MDL NUMBER: MFCD00375648

IUPAC: methyl 5-(methoxycarbonyl)-2,6-dimethyl-4-(4-nitrophenyl)-1,4-dihydropyridine-3-carboxylate

Smiles: C=1(C(C(=C(C)NC1C)C(=O)OC)c1ccc([N+](=[O-])=O)cc1)C(=O)OC

REFERENCE: Corburn, R. et. al. 1, 4-Dihydropyridine antagonist activities at the calcium channel: a quantitative structure-activity Relationship Aproach. J. Med. Chem. 1988,31, 2103-2107

ACCEPTORS: 6

DONORS: 1

ROTATION BONDS: 4

N+O: 8

Chiral Centers: 0

LogP: 3.56

LogS: -4.45

LIPINSKI: 4

