



Formula: C<sub>22</sub>H<sub>29</sub>NO<sub>5</sub>

MW: 387.48

CAS: 39133-31-8

MDL NUMBER: MFCD00133873

IUPAC: 2-(dimethylamino)-2-phenylbutyl 3,4,5-trimethoxybenzoate

Smiles: C(C(N(C)C)(CC)c1ccccc1)OC(=O)c1cc(OC)c(c(c1)OC)OC

Used to treat symptoms of irritable bowel syndrome (spastic colon); post-intestinal surgery treatment

THERAPEUTIC CATEGORY: Antispasmodic

ACCEPTORS: 5

DONORS: 0

ROTATION BONDS: 6

N+O: 6

Chiral Centers: 1

LogP: 4.78

LogS: -5.25

LIPINSKI: 4

Synonyms:

TRIMEBUTIN;TRIMEBUTINE;3,4,5-TRIMETHOXYBENZOATE,-2'-PHENYL-2'-DIMETHYLAMI  
NO-N-BUTYL;3,4,5-TRIMETHOXYBENZOIC ACID 2-[DIMETHYLAMINO]-2-PHENYLBUTYL  
ESTER;2'-PHENYL-2'-DIMETHYLAMINO-N-BUTYL-3',4',5'-TRIMETHOXYBENZOATE;trimebut  
ine free base;Trimebutine  
hydrochloride;TRIMEBUTINE3.4.5-TRIMETHOXYBENZOATE,-2'-PHENYL-2'-DIMETHYLAMIN  
O-N-BUTYL

CAS:39133-31-8

MF:C22H29NO5

MW:387.47

EINECS:254-309-2

Product Categories:ACTIVE PHARMACEUTICAL INGREDIENTS;API 3,4,5-Trimethoxybenzoic  
acid 2-(dimethylamino)-2-phenylbutyl ester

Chemical Properties: storage temp. 2-8C

CAS DataBase Reference: 39133-31-8(

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Safety Information: WGK Germany 3 3,4,5-Trimethoxybenzoic acid  
2-(dimethylamino)-2-phenylbutyl ester 3,4,5-Trimethoxybenzoic acid  
2-(dimethylamino)-2-phenylbutyl ester

Usage And Synthesis: 3,4,5-Trimethoxybenzoic acid 2-(dimethylamino)-2-phenylbutyl ester

