



Formula: C₂₄H₂₉N₃O₆

MW: 455.51

CAS: 57432-61-8

TNP NUMBER: TNP00154

MDL NUMBER: MFCD00078588

Smiles:

C1N(C)[C@@H]2(Cc3c4c(C2=C[C@H]1C(=O)N[C@H](CO)CC)cccc4[nH]c3).C(=C/C(=O)O)/C(=O)O

THERAPEUTIC CATEGORY: Oxytoxic

SOURCE: (Senisynthetic ergot alkooid, methabolite of methysergide

ACCEPTORS: 6

DONORS: 5

ROTATION BONDS: 7

N+O: 9

Chiral Centers: 3

LogP: 3.61

LogS: -4.66

LIPINSKI: 4

Synonyms:

erezingen;maleicacid,methylergonovine;methergine;methylergobasinemaleate;methyl-ergonovine maleate(1:1);METHYLERGOMETRINE MALEATE;METHYLERGONOVINE MALEATE;METHYLERGONOVINE MALEATE SALT

CAS:57432-61-8

MF:C24H29N3O6

MW:455.5

EINECS:260-734-4

Product Categories:Intermediates & Fine Chemicals;Metabolites & Impurities;Pharmaceuticals
Methylergonovine maleate salt

Chemical Properties: mp 1720C (dec) solubility H2O: 25 mg/mL color white T Risk
Statements 23/24/25-62 Safety Statements 36/37/39-45 RIDADR UN 1544 6.1/PG 3 WGK
Germany 3 RTECS KE5500000 HazardClass 6.1(b) PackingGroup III Methylergonovine
maleate salt

Usage And Synthesis:

Chemical Properties: Crystalline Solid UsageA metabolite of Methysergide. Semisynthetic ergot
alkaloid. Oxytotic Methylergonovine maleate salt

