

Product Name: Butabindide oxalate

Catalog No.: 1323

Batch No.: 4

CAS Number: 185213-03-0

IUPAC Name: (2S)-[1-[(2S)-2-amino-1-oxobutyl]-N-butyl]-2,3-dihydro-1H-indole-2-carboxamide oxalate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₅N₃O₂·C₂H₂O₄·³/₄H₂O

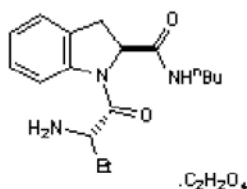
Batch Molecular Weight: 406.95

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol [9:1])

Melting Point: Between 124 - 126°C

HPLC: Shows >99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.08	7.06	10.33
Found	56.28	7.15	10.05

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Description:

High affinity, reversible, selective and competitive inhibitor of a CCK-inactivating serine protease (tripeptidyl peptidase II) ($K_i = 7$ nM). Active in vivo ($ID_{50} = 1.1$ and 6.8 mg/kg i.v. for inhibition of liver and brain enzyme respectively).

Physical and Chemical Properties:

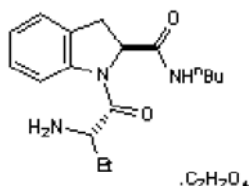
Batch Molecular Formula: $C_{17}H_{25}N_3O_2 \cdot C_2H_2O_4 \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 406.95

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at $-20^{\circ}C$

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

Sold with the permission of INSERM and UCL

References:

Ganellin et al (2000) Inhibitors of tripeptidyl peptidase II. 2. Generation of the first novel lead inhibitor of cholecystokinin-8-inactivating peptidase: a strategy for the design of peptidase inhibitors. *J.Med.Chem.* **43** 664. PMID: 10691692.

Renn et al (1998) Characterization and cloning of tripeptidyl peptidase II from the fruit fly, *Drosophila melanogaster*. *J.Biol.Chem.* **273** 19173. PMID: 9668104.

Rose et al (1996) Characterization and inhibition of a cholecystokinin-inactivating serine peptidase. *Nature* **380** 403. PMID: 8602240.

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