

## Product Information

### Compound Name

Sitagliptin EP Impurity B Phosphate Salt

### Synonyms

(3R)-3-amino-4-(2,5-difluorophenyl)-1-[3-(trifluoromethyl)-5H,6H,7H,8H-[1,2,4]triazolo[4,3-a]pyrazin-7-yl]butan-1-one; phosphoric acid

### Chemical Formula

C<sub>16</sub>H<sub>16</sub>OF<sub>5</sub>N<sub>5</sub>•H<sub>3</sub>O<sub>4</sub>P

### Molecular Weight

487.32

### Catalogue Number

S0006.114

### Lot No.

EDS-143-13

### Long-Term Storage Conditions

2-8°C

### Shipping Conditions

Ambient

### Appearance

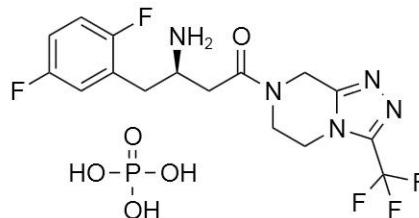
White Solid

### Method for Determining Identity

MS, <sup>1</sup>H NMR (D<sub>2</sub>O), <sup>13</sup>C NMR (DMSO-d<sub>6</sub>), HMBC, NOESY, HSQC

**Test Date:** Dec. 12, 2023

**Re-test Date:** Dec. 11, 2026



CAS No. : 1345822-87-8

## Analytical Information

### Solubility

CH<sub>3</sub>CN+H<sub>2</sub>O

### Elemental Analysis

Theoretical Value(%): C:39.43 H:3.93 N:14.37

Experimental Value(%): C:39.27 H:4.71 N:14.21

### Residual Solvents

No significant amounts of residual solvents were detected (<0.05%)

### Water Determination

0.19%(KF)

### Purity (HPLC)

98.26%

### Optical Rotation

[α]<sub>D</sub><sup>20.0</sup>(c=1.0000, H<sub>2</sub>O): -22.09°

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