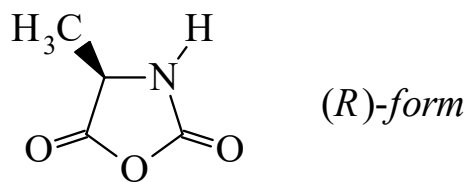




>>Entry Name: 4-Methyl-2,5-oxazolidinedione, 9CI

Synonym(s): *N*-Carboxyalanine anhydride. Alanine *N*-Carboxyanhydride. Ala-NCA



CAS Registry Number: 30291-41-9

Molecular Formula: C<sub>4</sub>H<sub>5</sub>NO<sub>3</sub>

Molecular Weight: 115.088

Accurate Mass: 115.026944

Percentage Composition: C 41.75%; H 4.38%; N 12.17%; O 41.71%

Use/Importance: Protected form of Alanine [BDL65-D](#) useful in the synth of peptides. Monomer for prepn. of poly(alanine)

Other Data: Unstable to acid

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 4829-14-5

Molecular Formula: C<sub>4</sub>H<sub>5</sub>NO<sub>3</sub>

Molecular Weight: 115.088

Accurate Mass: 115.026944

Percentage Composition: C 41.75%; H 4.38%; N 12.17%; O 41.71%

Physical Description: Solid (C<sub>6</sub>H<sub>6</sub>)

Sigma: J5293

>>Derivative: *N*-Benzyloxycarbonyl

CAS Registry Number: 129288-48-8

Molecular Formula: C<sub>12</sub>H<sub>11</sub>NO<sub>5</sub>

Molecular Weight: 249.223

Accurate Mass: 249.063724

Percentage Composition: C 57.83%; H 4.45%; N 5.62%; O 32.10%

Use/Importance: Highly effective reagent for peptide synth.

Physical Description: Cryst.

Melting Point: Mp 103-104.5°

Optical Rotation:  $[\alpha]_D^{25} -52.1$

Other Data: Unstable in H<sub>2</sub>O

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 2224-52-4

Molecular Formula: C<sub>4</sub>H<sub>5</sub>NO<sub>3</sub>

Molecular Weight: 115.088

Accurate Mass: 115.026944

Percentage Composition: C 41.75%; H 4.38%; N 12.17%; O 41.71%

Source/Synthesis: Used in the synth. of peptides and poly( $\alpha$ -amino acids)

Physical Description: Cryst. (Et<sub>2</sub>O/THF)

Melting Point: Mp 92° (90 dec.)

Optical Rotation:  $[\alpha]_D^{25} -2.7$  (c, 6.4 in dioxane)

>>Derivative: *N*-tert-Butoxycarbonyl

CAS Registry Number: 129288-31-9

Molecular Formula: C<sub>9</sub>H<sub>13</sub>NO<sub>5</sub>

Molecular Weight: 215.205

Accurate Mass: 215.079374

Percentage Composition: C 50.23%; H 6.09%; N 6.51%; O 37.17%

Use/Importance: Highly effective reagent for peptide synth.

Physical Description: Cryst.

Melting Point: Mp 103-104.5°

Optical Rotation:  $[\alpha]_D^{25} +21.6$

Other Data: Unstable in H<sub>2</sub>O

>>Variant: ( $\pm$ )-form