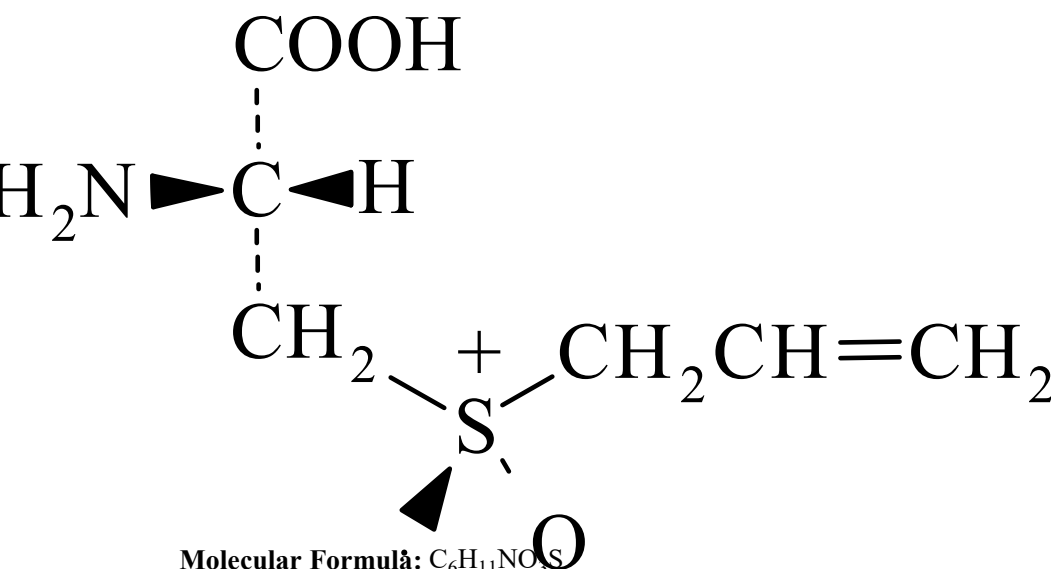




>>Entry Name: Alliin

ENTRY UNDER REVIEW

Synonym(s): 3-(2-Propenylsulfinyl)alanine, 9Cl. β -Allysulfenylalanine. *S*-Allylcysteine sulfoxide



Absolute
configuration

Molecular Formula: C₆H₁₁NO₃S

Molecular Weight: 177.224

Accurate Mass: 177.045964

Percentage Composition: C 40.66%; H 6.26%; N 7.90%; O 27.08%; S 18.09%

>>Variant: (*R*)_C(*S*)_S-form

CAS Registry Number: 556-27-4

Molecular Formula: C₆H₁₁NO₃S

Molecular Weight: 177.224

Accurate Mass: 177.045964

Percentage Composition: C 40.66%; H 6.26%; N 7.90%; O 27.08%; S 18.09%

Biological Source: Constit. of garlic oil (*Allium sativum*), also from ramsons (*Allium ursinum*)

Physical Description: Needles (Me₂CO aq.)

Melting Point: Mp 163 dec.°

Optical Rotation: [α]_D²¹+67.7 (c, 2.0 in H₂O)

Other Data: Other stereoisomers have been prepared synthetically