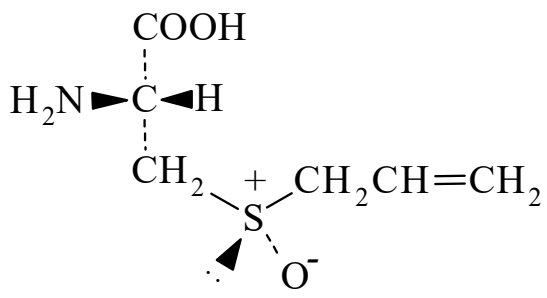
>>**Entry Name: Alliin**
ENTRY UNDER REVIEW
Synonym(s): 3-(2-Propenylsulfinyl)alanine, 9Cl. β-Allysulfenylalanine. *S*-Allylcysteine sulfoxide



Absolute configuration

Molecular Formula: $C_6H_{11}NO_3S$
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: $C_6H_{11}NO_3S$
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 (Me_2CO aq.)
Melting Point: Mp 163 dec.°
Optical Rotation: $[\alpha]_D^{21}$+67.7 (c, 2.0 in H_2O)
Other Data: Other stereoisomers have been prepared synthetically

>>**Derivative:** *N*-(1-Deoxy-β-D-fructopyranosyl)

CAS Registry Number: 149340-22-7

Molecular Formula: $C_{12}H_{21}NO_8S$
Molecular Weight: 339.366
Accurate Mass: 339.098789
Percentage Composition: C 42.47%; H 6.24%; N 4.13%; O 37.72%; S 9.45%
Biological Source: Isol. from garlic (*Allium sativum*)
Physical Description: Powder
Optical Rotation: $[\alpha]_D^{20}$–25.4 (c, 0.41 in H_2O)

>>**Derivative:** *N*-Ac

CAS Registry Number: 38131-20-3
Molecular Formula: $C_8H_{13}NO_4S$
Molecular Weight: 219.261
Percentage Composition: C 43.82%; H 5.98%; N 6.39%; O 29.19%; S 14.62%
Melting Point: Mp 188-198 dec.°
Optical Rotation: $[\alpha]_D^{21}$–29 (c, 1.0 in MeOH)

>>**Derivative:** *N*-Benzoyl

Molecular Formula: $C_{13}H_{15}NO_4S$
Molecular Weight: 281.332
Percentage Composition: C 55.50%; H 5.37%; N 4.98%; O 22.75%; S 11.40%
Melting Point: Mp 152-153.5 dec.°
Optical Rotation: $[\alpha]_D^{20}$–6 (c, 1.0 in MeOH)

>>**Derivative:** *N*-(4-Nitrobenzoyl)

Molecular Formula: $C_{13}H_{14}N_2O_6S$
Molecular Weight: 326.329
Accurate Mass: 326.057258
Percentage Composition: C 47.85%; H 4.32%; N 8.58%; O 29.42%; S 9.83%
Melting Point: Mp 180-182 dec.°
Optical Rotation: [α]