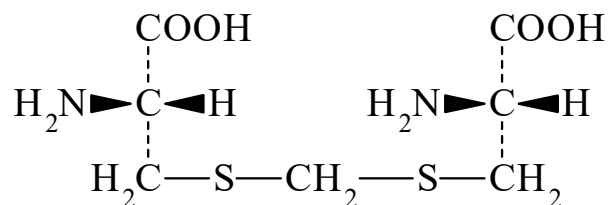




>>Entry Name: Djenkolic acid

Synonym(s): *S,S'*-Methylenebiscysteine, 9Cl



Molecular Formula: C₇H₁₄N₂O₄S₂

Molecular Weight: 254.331

Accurate Mass: 254.039498

Percentage Composition: C 33.06%; H 5.55%; N 11.01%; O 25.16%; S 25.22%

Sigma: D9255

>>Variant: (*R,R*)-form

Synonym(s): L-form

CAS Registry Number: 498-59-9

Type of Compound Code(s): VV0100 AH0100

Molecular Formula: C₇H₁₄N₂O₄S₂

Molecular Weight: 254.331

Accurate Mass: 254.039498

Percentage Composition: C 33.06%; H 5.55%; N 11.01%; O 25.16%; S 25.22%

Biological Source: Constit. of Djenkol bean (*Pithecolobium lobatum*). Also from *Abizia lophantha* and *Acacia* spp.

Physical Description: Needles (H₂O or HCl)

Melting Point: Mp 300-350 dec.°

Optical Rotation: [α]_D²⁰ -65 (c, 1 in HCl)

Other Data: Forms THF solvate, Mp 72-73.5°

>>Derivative: Hydrochloride

CAS Registry Number: 4508-48-9

Melting Point: Mp 250-300 dec.°

>>Derivative: *S*-Oxide

Synonym(s): 3-[[[(2-Amino-2-carboxyethyl)thio]methyl]sulfinyl]alanine, 8Cl. **Djenkolic acid sulfoxide**

CAS Registry Number: 21631-29-8

Type of Compound Code(s): VV0100 AH0100

Molecular Formula: C₇H₁₄N₂O₅S₂

Molecular Weight: 270.33

Accurate Mass: 270.034413

Percentage Composition: C 31.10%; H 5.22%; N 10.36%; O 29.59%; S 23.72%

Biological Source: Isol. from the seeds of *Acacia* spp.

>>Derivative: *S,S'*-Dioxide

Synonym(s): 3,3'-(Methylenedisulfinyl)dialanine, 8Cl. **Djenkolic acid disulfoxide**

CAS Registry Number: 20584-40-1

Type of Compound Code(s): VV0100 AH0100

Molecular Formula: C₇H₁₄N₂O₆S₂

Molecular Weight: 286.329

Accurate Mass: 286.029328

Percentage Composition: C 29.36%; H 4.93%; N 9.78%; O 33.53%; S 22.40%

Biological Source: Isol. from the seeds of *Acacia salicina*

>>Derivative: Di-Et ester

Molecular Formula: C₁₁H₂₂N₂O₄S₂

Molecular Weight: 310.438

Accurate Mass: 310.102098

Percentage Composition: C 42.56%; H 7.14%; N 9.02%; O 20.62%; S 20.66%

Physical Description: Cryst. (EtOH) (as dihydrochloride)

Melting Point: Mp 171-173° (dihydrochloride)

Optical Rotation: [α]_D²⁵ -40 (c, 1 in DMF)

Other Data: Forms THF solvate, Mp 72-73.5°