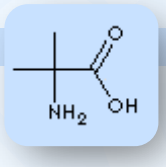
alpha-AMINOISOBUTYRIC ACID

SYNONYMS

2-Aminoisobutyric acid; 2-Amino-2-methylpropanoic acid; 2-Aminoisobutyric acid; 2-Methylalanine; AIB; alpha,alpha-Dimethylglycine; alpha-Aminoisobutanoic acid; alpha-Methylalanine; 2-Amino-2-methylpropionic acid;



PRODUCT IDENTIFICATION

CAS RN	62-57-7; 18389-23-6; 765258-64-8
EINECS RN	200-544-0
FORMULA	$(CH_3)_2C(NH_2)COOH$
MOL WEIGHT	103.12

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	white crystalline powder
MELTING POINT	335 C
BOILING POINT	
DENSITY	
SOLUBILITY IN WATER	Soluble (practically insoluble in alcohol, insoluble in ether)
pH	
VAPOR DENSITY	
REFRACTIVE INDEX	
FLASH POINT	

GENERAL DESCRIPTION & APPLICATION

Protein function is governed by physical characteristics such as flexibility and structure. The formation of secondary and tertiary structures is accomplished through the interaction of atoms and accompanying weak forces, which ultimately control protein flexibility. One of the most important weak forces is the hydrogen bond, which is found to occur between backbone atoms in secondary structures such as helices, sheets and coils. The most common helix conformation is the alpha-helix, characterized by an (i -> i + 4) hydrogen bonding pattern. A less common helix structure, sometimes found in protein binding sites and possibly as an intermediate during alpha-helical formation, is the 310-helix (characterized by an (i -> i + 3) hydrogen bonding pattern). It has been found that peptides primarily composed of the amino acid Aib (alpha-aminoisobutyric acid) will readily fold into 310-helices, even in peptides as short as three residues. Aib amino acids are structurally similar to alanine except for a methyl group in place of a hydrogen at the alpha-carbon. The dialkylation at the alpha-carbon creates significant steric hindrance, which is responsible for the helical preference of Aib. We are interested in the role that steric hidrance plays in governing helical structure and flexibility. The peptide of interest in this study is an eight residue chain with alanine amino acids at positions three and six and Aib residues at the remaining positions ("AA36"). Since Aib is sterically hindered and will drive the formation of a 310-helix, the two alanine residues will create two less sterically hindered and presumably more flexible regions of the helix. In this project, the AA36 peptide is prepared using solution phase synthesis, and 1H NMR is used to study amide proton exchange with deuterons in the solvent to characterize helical flexibility. The analysis of this data and comparison to that for similar peptides will lend insight to the role of steric hinderance and hydrogen bond strength in helix flexibility. (source: http://www.dep.anl.gov/)

Tripeptides of formula (I) and their salts wherein X is an amino acid residue linked, at its carboxyl group, to the amino group of L-aspartic acid through peptide bonding; Asp denotes an L-aspartic acid residue which is linked, at its amino group, to the amino acid residue X through peptide bonding and is connected, at its carboxyl group attached to the amino-substituted carbon atom, to the amino acid residue Y through peptide bonding; Y is an amino acid residue which is linked, at its amino group, to Asp through peptide bonding and is connected, at its carboxyl group, to an alcohol through ester bonding; OR is an alcohol residue linked, at its hydroxyl-group, to the amino acid residue Y through ester bond-ing;

alpha-AMINOISOBUTYRIC ACID

R is alkyl or cyclo alkyl; the amino acid residue X is a D- or DL-isomer except when it is glycine or .alpha.-amino-isobutyric acid; and the amino acid residue Y is an L-, D- or DL-isomer when it is not an amino acid having no center of optical activity, are suitable as sweeteners exhibiting soft sweetness. (source: http://patents.ic.gc.ca/)

Ca,a-disubstituted amino acids (aaAA) are a class of non-coded amino acids in which the presence of two substitutents (usually alkyl groups) at the a-carbon imposes intense constraints on the φ/ψ angles of the residue (Figure 1.7). The most commonly studied aaAA is certainly a-aminoisobutyric acid (Aib). Aib is a naturally occurring amino acid produced by microbial sources,1.1-1.4 typically by non-ribosomal peptide synthesis. It is known that Aib residues have dramatic influences on peptide backbone conformation.1.16-1.20 In an Aib residue, the rotation about N-Ca and Ca-C' bond is restricted. The energy minimum for the dihedral angle φ and ψ of Aib occur near ?57°, -47° and 57°, 47° respectively, which corresponds to a right-handed or left-handed a-helix or 310-helix in Ramachandran plot.1.18, 1.21-1.22 Early studies on alamethicin crystal structure by Fox and Richards showed this Aib-containing peptide adopted a mixture of 310- and a-helical structures in the solid state.1.23 Since the 1980s, a number of groups such as Balaram's and Toniolo's group, have done extensive studies on Aib peptide conformation.1.16, 1.18-1.19 Studies have shown that Aib peptides can adopt a, 310 or a/310-helical structures depending on sequence length, Aib content, and solvent effects.1.7, 1.18,1.24 It has been reported that the minimal length for a peptide to form an a-helix is seven residues, while no significant chain length is required for 310-helix formation. Peptides with more than 8 residues are more likely to adopt an a-helix than a 310-helix, if the Aib residue content is not more than 50%. Meanwhile, even a single a-helix chain often has 310-helices present at either end of the stretch which tightens up the ends of the a-helix structure.1.10 It has been found that solvents also effect the conformational preference of Aib rich peptides.1.5, 1.7, 1.25 In peptides where the a/310-helix equilibrium exists, solvents with high polarity usually favor the a-helix formation, while the 310-helix is often found in low polarity solvent systems. (source: http://etd.lsu.edu/)

STABILITY AND REACTIVITY

STABILITY	Stable under normal conditions.
CONDITIONS OF INSTABILITY	
INCOMPATIBLE MATERIALS	Strong oxidizing agents.
DECOMPOSITION PRODUCTS	Nitrogen oxides, carbon monoxide, carbon monoxide, carbon dioxide, nitrogen gas
POLYMERIZATION	Will not occur

SAFETY

HAZARD NOTES	Irritant. Irritating to eyes, respiratory system and skin.
EYE	May cause eye irritation.
SKIN	May cause skin irritation.
INGESTION	May cause irritation of the digestive tract.
INHALATION	May cause respiratory tract irritation.
CHRONIC	
NFPA RATING	Health: , Flammability: , Reactivity:

SALES SPECIFICATION

APPEARANCE	white crystalline powder
ASSAY	99.0% min

TRANSPORT & REGULATORY INFORMATION

UN NO.

alpha-AMINOISOBUTYRIC ACID

HAZARD CLASS	
PACKING GROUP	
HAZARD SYMBOL	
RISK PHRASES	
SAFETY PHRASES	24/25

PACKING

PRICE