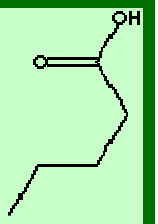
VALERIC ACID



PRODUCT IDENTIFICATION	
CAS NO.	109-52-4; 12124-87-7
EINECS NO.	203-677-2
FORMULA	$CH_3(CH_2)_3COOH$
MOL WT.	102.13
H.S. CODE	2915.60.9000
TOXICITY	Mouse LD50 (Oral): 600mg/kg
SYNONYMS	n-Pentanoic Acid; Butanecarboxylic Acid; Carboxylic acid C5; 1-Butanecarboxylic acid; Propylacetic acid; Valerianic acid; Kyselina Valerova (Czech);
SMILES	C(C(O)=O)CCC
CLASSIFICATION	Straight chain fatty acid, Flavors & Fragrances, Biochemical ex Plants

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	Clear, pale beige liquid
MELTING POINT	-33.5 C
BOILING POINT	186 C
SPECIFIC GRAVITY	0.934-0.939
SOLUBILITY IN WATER	10-50 mg/ml (soluble in ethanol, ethyl ether)
VAPOR DENSITY	
pKa	4.84 (Dissociation Constant at 20 C)
log Pow	1.39 (Octanol-water)
VAPOR PRESSURE	0.196 (mmHg at 25 C)
HENRY'S LAW	4.72E-07 (atm-m3/mole at 25 C)
OH RATE	4.11E-12 (cm3/molecule-sec at 25 C Atmospheric)
NFPA RATINGS	Health ; 2 Flammability ; 1 Reactivity ; 0
REFRACTIVE INDEX	1.405-1.414
FLASH POINT	95 C
STABILITY	Stable under ordinary conditions

GENERAL DESCRIPTION & EXTERNAL LINKS

Valeric acid (pentanoic acid or propylacetic acid in systemic naming) is a member of short chain straight fatty acids. It is a colorless liquid with a penetrating aroma; slightly soluble in water, soluble in alcohol, and ether. It melts at -34 C and boils at 186 C . ; boils at 185 C . Isovaleric acid (3-methylbutanoic acid) is a member of branched fatty acids. It is a colorless liquid; slightly soluble in water, soluble in alcohol, and almost organic solvents including ethers. It has a strong pungent sweaty smell. It melts at -29 C and boils at 176 C. Their primary application is in the synthesis of its esters which are more volatile than their parent compounds. Valeric esters have distinctive fruit-like odors, which has led to the use in fruity flavors, perfume and cosmetics. (e.g: Methyl valerate:flowery, Ethyl valerate: fruity particularly apple, Ethyl isovalerate:apple, Amyl valerate: apple and pineapple).

There are almost infinite esters obtained from thousands of potential starting materials. Esters are formed by removal of water from an acid and an alcohol, e.g., carboxylic acid esters, phosphoric acid esters, and sulfonic acid esters. Carboxylic acid esters are used as in a variety of direct and indirect applications. Lower chain esters are used as flavouring base materials, plasticizers, solvent carriers and coupling agents. Higher chain compounds are used as components in metalworking fluids, surfactants, lubricants, detergents, oiling agents, emulsifiers, wetting agents textile treatments

and emollients, They are also used as intermediates for the manufacture of a variety of target compounds. The almost infinite esters provide a wide range of viscosity, specific gravity, vapor pressure, boiling point, and other physical and chemical properties for the proper application selections.

Valeric acid, isovaleric acid their esters are useful raw material for variety of industrial target compounds including;

- Plasticizers and Lubricants
- Biodegradable solvents and lubricants
- Engineering plastics
- Epoxy curing agents
- Adhesive and powder coatings
- Corrosion inhibitors
- Perfumery and pharmaceuticals
- Electrolytes

Vinyl stabilizers

SALES SPECIFICATION	
APPEARANCE	Clear, pale beige liquid
CONTENT	98.0% min
ACID VALUE	538 - 550 (mg KOH/g)
MOISTURE	0.5% max

TRANSPORTATION	
PACKING	190kgs in Drum
HAZARD CLASS	8
UN NO.	1760

GENERAL DESCRIPTION OF CARBOXYLIC ACID

Carboxylic acid is an organic compound whose molecules contain carboxyl group and have the condensed chemical formula R-C(=O)-OH in which a carbon atom is bonded to an oxygen atom by a solid bond and to a hydroxyl group by a single bond), where R is a hydrogen atom, an alkyl group, or an aryl group. Carboxylic acids can be synthesized if aldehyde is oxidized. Aldehyde can be obtained by oxidation of primary alcohol. Accordingly, carboxylic acid can be obtained by complete oxidation of primary alcohol. A variety of Carboxylic acids are abundant in nature and many carboxylic acids have their own trivial names. Examples are shown in table. In substitutive nomenclature, their names are formed by adding -oic acid' as the suffix to the name of the parent compound. The first character of carboxylic acid is acidity due to dissociation into H^+ cations and $RCOO^-$ anions in aqueous solution. The two oxygen atoms are electronegatively charged and the hydrogen of a carboxyl group can be easily removed. The presence of electronegative groups next to the carboxylic group increases the acidity. For example, trichloroacetic acid is a stronger acid than acetic acid. Carboxylic acid is useful as a parent material to prepare many chemical derivatives due to the weak acidity of the hydroxyl hydrogen or due to the difference in electronegativity between carbon and oxygen. The easy dissociation of the hydroxyl oxygen-hydrogen provide reactions to form an ester with an alcohol and to form a water-soluble salt with an alkali. Almost infinite esters are formed through condensation reaction called esterification between carboxylic acid and alcohol, which produces water. The second reaction theory is the addition of electrons to the electron-deficient carbon atom of the carboxyl group. One more theory is decarboxylation (removal of carbon dioxide form carboxyl group). Carboxylic acids are used to synthesize acyl halides and acid anhydrides which are generally not target compounds. They are used as intermediates for the synthesis esters and amides, important derivatives from carboxylic acid in biochemistry as well as in industrial fields. There are almost infinite esters obtained

from carboxylic acids. Esters are formed by removal of water from an acid and an alcohol. Carboxylic acid esters are used as in a variety of direct and indirect applications. Lower chain esters are used as flavouring base materials, plasticizers, solvent carriers and coupling agents. Higher chain compounds are used as components in metalworking fluids, surfactants, lubricants, detergents, oiling agents, emulsifiers, wetting agents textile treatments and emollients, They are also used as intermediates for the manufacture of a variety of target compounds. The almost infinite esters provide a wide range of viscosity, specific gravity, vapor pressure, boiling point, and other physical and chemical properties for the proper application selections. Amides are formed from the reaction of a carboxylic acids with an amine. Carboxylic acid's reaction to link amino acids is wide in nature to form proteins (amide), the principal constituents of the protoplasm of all cells. Polyamide is a polymer containing repeated amide groups such as various kinds of nylon and polyacrylamides. Carboxylic acid are in our lives.