

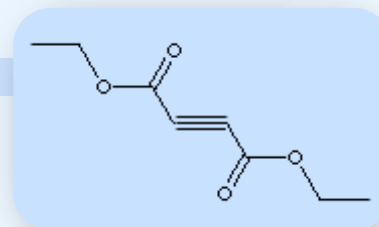
DIETHYL ACETYLENEDICARBOXYLATE

SYNONYMS

1,2-Bis(ethoxycarbonyl)acetylene; 1,2-Bis(ethoxycarbonyl)ethyne; Acetylenedicarboxylic acid, diethyl ester; Bis(ethoxycarbonyl)acetylene; Di(carboethoxy)acetylene; Diethyl 2-butynedioate; Diethyl acetylenedicarboxylic acid; Diethyl butynedioate; Diethyl ethynedicarboxylate; Ethyl acetylenedicarboxylate;

PRODUCT IDENTIFICATION

CAS RN	762-21-0
EINECS RN	212-098-4
FORMULA	C ₂ H ₅ OCOC≡CCOOC ₂ H ₅
MOL WEIGHT	170.16



PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	colorless to light yellow liquid
MELTING POINT	1 - 2 C
BOILING POINT	107 - 110 C at 11 mmHg
DENSITY	1.06 - 1.07
SOLUBILITY IN WATER	Insoluble (soluble in ethanol, ethyl ether, CCl ₄ , miscible with organic solvents)
pH	
VAPOR DENSITY	
REFRACTIVE INDEX	1.441 - 1.443
FLASH POINT	94 C

APPLICATION

1. Diels-Alder Reaction

The [4+2]-cycloaddition of a conjugated diene and a dienophile (an alkene or alkyne), an electrocyclic reaction that involves the 4 π-electrons of the diene and 2 π-electrons of the dienophile. The driving force of the reaction is the formation of new σ-bonds, which are energetically more stable than the π-bonds. In the case of an alkynyl dienophile, the initial adduct can still react as a dienophile if not too sterically hindered. In addition, either the diene or the dienophile can be substituted with cumulated double bonds, such as substituted allenes. With its broad scope and simplicity of operation, the Diels-Alder is the most powerful synthetic method for unsaturated six-membered rings. A variant is the hetero-Diels-Alder, in which either the diene or the dienophile contains a heteroatom, most often nitrogen or oxygen. This alternative constitutes a powerful synthesis of six-membered ring heterocycles. (source: <http://www.organic-chemistry.org/>)

2. Inhibitor of oxidative phosphorylation → pesticide

Some insecticides inhibit or disrupt energy production. Initially, the insect can mobilize enough stored energy to continue its basic functions. While it can eat and digest food in the initial stages after being poisoned, it cannot produce more energy from the food. Eventually, the insect "runs out of steam," stops eating and even moving, and dies. (source: <http://www.entmclasses.umd.edu/>)

Acetylenedicarboxylate compounds

Product	CAS RN.
2-Butynedioic acid	142-45-0
Cellocidin	543-21-5
Diethyl 2-butynedioate	762-21-0
Methyl acetylenedicarboxylate	762-42-5
Potassium hydrogen butynedioate	928-04-1



DIETHYL ACETYLENEDICARBOXYLATE

Dipropargyl acetylenedicarboxylate	3154-91-4
Di-tert-butyl 2-butyne dioate	66086-33-7
Bis(triphenyltin) acetylenedicarboxylate	73940-87-1

STABILITY AND REACTIVITY

STABILITY	Stable under normal conditions.
CONDITIONS OF INSTABILITY	
INCOMPATIBLE MATERIALS	Strong oxidizing agents, Strong acids, Strong bases, Strong reducing agents.
DECOMPOSITION PRODUCTS	Carbon monoxide, Carbon dioxide.
POLYMERIZATION	Will not occur

SAFETY

HAZARD NOTES	Causes burns. Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin. Inhalation may result in spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis, and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting. Exposure can cause: Nausea, headache, and vomiting. Cyanosis. Convulsions.
EYE	Material is extremely destructive to eye.
SKIN	Material is extremely destructive to skin.
INGESTION	Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract.
INHALATION	May result in spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis, and pulmonary edema
CHRONIC NFPA RATING	Health: 3, Flammability: 2, Reactivity: 0

SALES SPECIFICATION

APPEARANCE	colorless to light yellow liquid
ASSAY	98.0% min
REFRACTIVE INDEX	1.446 - 1.448

TRANSPORT & REGULATORY INFORMATION

UN NO.	3265
HAZARD CLASS	8
PACKING GROUP	II
HAZARD SYMBOL	C
RISK PHRASES	34
SAFETY PHRASES	23-26-27-36/37/39-45

PACKING

PRICE

