

ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

Page: 1

Compilation date: 11/11/2010

Revision No: 1

# Section 1: Identification of the substance/mixture and of the company/undertaking

# 1.1. Product identifier

Product name: ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

CAS number: 3516-87-8

Product code: PC5767

Synonyms: ETHYL (PENTAFLUOROBENZOYL)ACETATE

ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPIONATE

# 1.2. Relevant identified uses of the substance or mixture and uses advised against

## 1.3. Details of the supplier of the safety data sheet

Company name: Apollo Scientific Ltd

	Units 3 & 4
	Parkway
	Denton
	Manchester
	M34 3SG
	UK
Tel:	0161 337 9971
Fax:	0161 336 6932
Email:	david.tideswell@apolloscientific.co.uk

# 1.4. Emergency telephone number

# Section 2: Hazards identification

# 2.1. Classification of the substance or mixture

Classification under CHIP:	-: R10; Xn: R20/21/22; Xi: R36/37/38	
Classification under CLP: STOT SE 3: H335; Acute Tox. 4: H302+312+332; Eye Irrit. 2: H319; Flam. Liq. 3: H226;		
	Skin Irrit. 2: H315	
Most important adverse effects:	Flammable. Harmful by inhalation, in contact with skin and if swallowed. Irritating to	
	eyes, respiratory system and skin.	

# 2.2. Label elements

Label elements under CLP:

Hazard statements: H226: Flammable liquid and vapour.

H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.

H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

## ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

Signal words: Warning Hazard pictograms: GHS02: Flame GHS07: Exclamation mark Precautionary statements: P280: Wear protective gloves/protective clothing/eye protection/face protection. P210: Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Label elements under CHIP: Hazard symbols: Harmful. Risk phrases: R10: Flammable. R20/21/22: Harmful by inhalation, in contact with skin and if swallowed. R36/37/38: Irritating to eyes, respiratory system and skin. Safety phrases: S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S36/37/39: Wear suitable protective clothing, gloves and eye / face protection. S45: In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). 2.3. Other hazards

Other hazards: In use, may form flammable / explosive vapour-air mixture.

**PBT:** This substance is not identified as a PBT substance.

# Section 3: Composition/information on ingredients

# 3.1. Substances

Chemical identity: ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

# Section 4: First aid measures

## 4.1. Description of first aid measures

Skin contact:	Remove all contaminated clothes and footwear immediately unless stuck to skin.		
	Drench the affected skin with running water for 10 minutes or longer if substance is still		
	on skin. Consult a doctor.		
Eye contact:	Bathe the eye with running water for 15 minutes. Consult a doctor.		
Ingestion:	Wash out mouth with water. Do not induce vomiting. If conscious, give half a litre of water		
	to drink immediately. Consult a doctor.		
Inhalation:	Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a		
	doctor.		

ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

4.2. Most important symptoms	and effects, both acute and delayed		
Skin contact:	There may be irritation and redness at the site of contact.		
Eye contact:	There may be irritation and redness. The eyes may water profusely.		
Ingestion:	There may be soreness and redness of the mouth and throat. Nausea and stomach		
	pain may occur. There may be vomiting.		
Inhalation:	There may be irritation of the throat with a feeling of tightness in the chest.		
4.3. Indication of any immediate	e medical attention and special treatment needed		
Occien 5. Eiro fighting mooou			
Section 5: Fire-fighting measur	res		
5.1. Extinguishing media			
Extinguishing media:	Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the		
	surrounding fire should be used. Use water spray to cool containers.		
5.2. Special hazards arising fro	m the substance or mixture		
	Flammable. Forms explosive air-vapour mixture. In combustion emits toxic fumes.		
Exposure nazarus.			
	Carbon oxides. Hydrogen fluoride (HF).		
5.3. Advice for fire-fighters			
Advice for fire-fighters:	Wear self-contained breathing apparatus. Wear protective clothing to prevent contact		
	with skin and eyes.		
Section 6: Accidental release n	neasures		
6.1. Personal precautions, prot	ective equipment and emergency procedures		
Personal precautions:	Refer to section 8 of SDS for personal protection details. If outside do not approach from		
· · · · · · · · · · · · · · · · · · ·	downwind. If outside keep bystanders upwind and away from danger point. Mark out the		
	contaminated area with signs and prevent access to unauthorised personnel. Turn		
	leaking containers leak-side up to prevent the escape of liquid. Eliminate all sources of		
	ignition.		
6.2. Environmental precautions	-		
<u>-</u>			
-	Do not discharge into drains or rivers. Contain the spillage using bunding.		
6.3. Methods and material for c	ontainment and cleaning up		
Clean-up procedures:	Absorb into dry earth or sand. Transfer to a closable, labelled salvage container for		
	disposal by an appropriate method. Do not use equipment in clean-up procedure which		
	may produce sparks.		
6.4. Reference to other sections			
Section 7. Handling and store			
Section 7: Handling and storag	je		

# ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

7.1. Precautions for safe handling			
Handling requirements:	Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area.		
	Do not handle in a confined space. Avoid the formation or spread of mists in the air.		
	Smoking is forbidden. Use non-sparking tools. Only use in fume hood.		
7.2. Conditions for safe storage	e, including any incompatibilities		
Storage conditions:	Store in cool, well ventilated area. Keep container tightly closed. Keep away from		
	sources of ignition. Prevent the build up of electrostatic charge in the immediate area.		
	Ensure lighting and electrical equipment are not a source of ignition.		
Suitable packaging:	Must only be kept in original packaging.		
7.3. Specific end use(s)			
Specific end use(s):	No data available.		
Section 8: Exposure controls/p			
8.1. Control parameters			
Workplace exposure limits:	Not applicable.		
8.2. Exposure controls			
Engineering measures:	Ensure there is sufficient ventilation of the area. Ensure lighting and electrical		
	equipment are not a source of ignition.		
Respiratory protection:	Self-contained breathing apparatus must be available in case of emergency.		
	Impermeable gloves.		
-	Safety glasses. Ensure eye bath is to hand.		
	Impermeable protective clothing.		
Section 9: Physical and chemic			
-			
9.1. Information on basic physi	cal and chemical properties		
State:	Liquid		
Colour:	Colourless		

Flash point °C: 41

9.2. Other information

Other information: Not applicable.

Boiling point/range ℃: 103-104@4mmHg

Relative density: 1.43

# Section 10: Stability and reactivity

10.1. Reactivity

Reactivity: Stable under recommended transport or storage conditions.

10.2. Chemical stability

Chemical stability: Stable under normal conditions. Stable at room temperature.

Page: 4

## ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

## 10.3. Possibility of hazardous reactions

Hazardous reactions: Hazardous reactions will not occur under normal transport or storage conditions.

# 10.4. Conditions to avoid

Conditions to avoid: Heat. Hot surfaces. Sources of ignition. Flames.

#### 10.5. Incompatible materials

Materials to avoid: Strong oxidising agents. Strong acids.

# 10.6. Hazardous decomposition products

Haz. decomp. products: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Hydrogen fluoride

(HF).

#### Section 11: Toxicological information

## 11.1. Information on toxicological effects

#### Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	INH DRM ING	Based on test data
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data
STOT-single exposure	INH	Based on test data

## Symptoms / routes of exposure

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach

pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

# Section 12: Ecological information

#### 12.1. Toxicity

Ecotoxicity values: Not applicable.

# 12.2. Persistence and degradability

Persistence and degradability: No data available.

12.3. Bioaccumulative potential

Bioaccumulative potential: No data available.

12.4. Mobility in soil

Mobility: No data available.

# ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

# Page: 6 12.5. Results of PBT and vPvB assessment PBT identification: This substance is not identified as a PBT substance. 12.6. Other adverse effects Other adverse effects: No data available. Section 13: Disposal considerations 13.1. Waste treatment methods Disposal operations: MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS Disposal of packaging: Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations. **NB:** The user's attention is drawn to the possible existence of regional or national regulations regarding disposal. Section 14: Transport information 14.1. UN number UN number: UN3272 14.2. UN proper shipping name Shipping name: ESTERS, N.O.S. 14.3. Transport hazard class(es) Transport class: 3 14.4. Packing group Packing group: III 14.5. Environmental hazards Environmentally hazardous: No Marine pollutant: No 14.6. Special precautions for user Tunnel code: D/E Transport category: 3 Section 15: Regulatory information 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture 15.2. Chemical Safety Assessment Chemical safety assessment: A chemical safety assessment has not been carried out for the substance or the mixture by the supplier. Section 16: Other information

# ETHYL 3-OXO-3-(PENTAFLUOROPHENYL)PROPANOATE 98%

Other information		
Other information:	: This safety data sheet is prepared in accordance with Commission Regulation (EU) No	
	453/2010.	
	* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by	
	decision tree approach. http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?	
	c=TOXTREE	
	<ul> <li>Data predicted using computatioanl software ACD/ToxSuite v 2.95.1 Copyright 1994-</li> </ul>	
	2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry	
	Development, Inc (ACD/Labs). http://www.acdlabs.com/products/pc_admet/tox/tox/	
Dhrasos used in s 2 and 2:	H226: Flammable liquid and vapour.	
Fillases used in S.2 and S.	H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.	
	H315: Causes skin irritation.	
	H319: Causes serious eye irritation.	
	H335: May cause respiratory irritation.	
	R10: Flammable.	
	R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.	
	R36/37/38: Irritating to eyes, respiratory system and skin.	
Legal disclaimer:	The material is intended for research purposes only and should be handled exclusively	
	by those who have been fully trained in safety, laboratory and chemical handling	
	procedures. The above information is believed to be correct to the best of our	
	knowledge. The above information is believed to be correct to the best of our knowledge	
	at the date of its publication, but should not be considered to be all inclusive. It should	
	be used only as a guide for safe handling, storage, transportation and disposal. We	
	cannot guarantee that the hazards detailed in this document are the only hazards that	
	exist for this product. This is not a warranty and Apollo Scientific Ltd shall not be held	
	liable for any damage resulting from handling or from contact with the above product.	
	name for any damage resulting from handling of from contact with the above product.	