



## SAFETY DATA SHEET

### 4-(Trifluoromethoxy)aniline

According to Regulation (EC) No 1907/2006, Annex II, as amended. Commission Regulation (EU) No 2015/830 of 28 May 2015.

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

##### 1.1. Product identifier

Product name	4-(Trifluoromethoxy)aniline
Product number	59603501
CAS number	461-82-5
EC number	207-317-5

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

Uses advised against	For research and development purposes. Not suitable for human consumption or veterinary purposes.
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##### 1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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##### 1.4. Emergency telephone number

+44 (0) 1380 725952

#### SECTION 2: Hazards identification

##### 2.1. Classification of the substance or mixture

###### Classification (EC 1272/2008)

Physical hazards	Not Classified
Health hazards	Acute Tox. 3 - H301 Acute Tox. 2 - H310 Acute Tox. 2 - H330 Skin Irrit. 2 - H315 Eye Dam. 1 - H318 STOT RE 2 - H373
Environmental hazards	Aquatic Chronic 3 - H412

##### 2.2. Label elements

EC number	207-317-5
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###### Hazard pictograms



Signal word

Danger

## 4-(Trifluoromethoxy)aniline

<b>Hazard statements</b>	<p>H301 Toxic if swallowed.</p> <p>H310+H330 Fatal in contact with skin or if inhaled.</p> <p>H315 Causes skin irritation.</p> <p>H318 Causes serious eye damage.</p> <p>H373 May cause damage to organs through prolonged or repeated exposure.</p> <p>H412 Harmful to aquatic life with long lasting effects.</p>
<b>Precautionary statements</b>	<p>P260 Do not breathe vapour/ spray.</p> <p>P262 Do not get in eyes, on skin, or on clothing.</p> <p>P264 Wash contaminated skin thoroughly after handling.</p> <p>P271 Use only outdoors or in a well-ventilated area.</p> <p>P273 Avoid release to the environment.</p> <p>P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.</p> <p>P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.</p> <p>P302+P352 IF ON SKIN: Wash with plenty of water.</p> <p>P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.</p> <p>P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.</p> <p>P314 Get medical advice/ attention if you feel unwell.</p> <p>P330 Rinse mouth.</p> <p>P332+P313 If skin irritation occurs: Get medical advice/ attention.</p> <p>P361+P364 Take off immediately all contaminated clothing and wash it before reuse.</p> <p>P362+P364 Take off contaminated clothing and wash it before reuse.</p> <p>P403+P233 Store in a well-ventilated place. Keep container tightly closed.</p> <p>P405 Store locked up.</p> <p>P501 Dispose of contents/ container in accordance with national regulations.</p>

### 2.3. Other hazards

This substance is not classified as PBT or vPvB according to current EU criteria.

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

<b>Product name</b>	4-(Trifluoromethoxy)aniline
<b>CAS number</b>	461-82-5
<b>EC number</b>	207-317-5
<b>Chemical formula</b>	CF <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

<b>General information</b>	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
<b>Inhalation</b>	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention. Place unconscious person on their side in the recovery position and ensure breathing can take place.
<b>Ingestion</b>	Get medical attention immediately. Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation.

## 4-(Trifluoromethoxy)aniline

<b>Skin contact</b>	It is important to remove the substance from the skin immediately. Remove contamination with soap and water or recognised skin cleansing agent. Get medical attention.
<b>Eye contact</b>	Rinse immediately with plenty of water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Continue to rinse for at least 15 minutes and get medical attention.
<b>Protection of first aiders</b>	It may be dangerous for first aid personnel to carry out mouth-to-mouth resuscitation.

### **4.2. Most important symptoms and effects, both acute and delayed**

<b>General information</b>	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
<b>Inhalation</b>	A single exposure may cause the following adverse effects: Difficulty in breathing. Unconsciousness, possibly death.
<b>Ingestion</b>	May cause stomach pain or vomiting. May cause severe internal injury.
<b>Skin contact</b>	A single exposure may cause the following adverse effects: Pain. Unconsciousness, possibly death.
<b>Eye contact</b>	Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.

### **4.3. Indication of any immediate medical attention and special treatment needed**

<b>Notes for the doctor</b>	Treat symptomatically. Keep affected person under observation.
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## **SECTION 5: Firefighting measures**

### **5.1. Extinguishing media**

<b>Suitable extinguishing media</b>	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
<b>Unsuitable extinguishing media</b>	Do not use water jet as an extinguisher, as this will spread the fire.

### **5.2. Special hazards arising from the substance or mixture**

<b>Specific hazards</b>	Containers can burst violently or explode when heated, due to excessive pressure build-up. This product is toxic.
<b>Hazardous combustion products</b>	Thermal decomposition or combustion products may include the following substances: Very toxic or corrosive gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO <sub>2</sub> ). Nitrous gases (NO <sub>x</sub> ). Hydrogen fluoride (HF).

### **5.3. Advice for firefighters**

<b>Protective actions during firefighting</b>	Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. If a leak or spill has not ignited, use water spray to disperse vapours and protect men stopping the leak. Avoid discharge to the aquatic environment. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.
<b>Special protective equipment for firefighters</b>	Wear chemical protective suit. Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents.

## **SECTION 6: Accidental release measures**

## 4-(Trifluoromethoxy)aniline

### 6.1. Personal precautions, protective equipment and emergency procedures

**Personal precautions** Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of vapours and spray/mists. Use suitable respiratory protection if ventilation is inadequate. Avoid contact with skin and eyes.

### 6.2. Environmental precautions

**Environmental precautions** Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

### 6.3. Methods and material for containment and cleaning up

**Methods for cleaning up** Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Provide adequate ventilation. Small Spillages: Collect spillage. Large Spillages: Absorb spillage with non-combustible, absorbent material. The contaminated absorbent may pose the same hazard as the spilled material. Collect and place in suitable waste disposal containers and seal securely. Label the containers containing waste and contaminated materials and remove from the area as soon as possible. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. For waste disposal, see Section 13.

### 6.4. Reference to other sections

**Reference to other sections** For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

**Usage precautions** Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Handle all packages and containers carefully to minimise spills. Keep container tightly sealed when not in use. Avoid the formation of mists. This product is toxic. Immediate first aid is imperative. Avoid discharge to the aquatic environment. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

**Advice on general occupational hygiene** Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

### 7.2. Conditions for safe storage, including any incompatibilities

**Storage precautions** Store away from incompatible materials (see Section 10). Store locked up. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

**Storage class** Toxic storage.

### 7.3. Specific end use(s)

**Specific end use(s)** The identified uses for this product are detailed in Section 1.2.

## SECTION 8: Exposure controls/Personal protection

### 8.1. Control parameters

STEL

TWA

### 8.2. Exposure controls

## 4-(Trifluoromethoxy)aniline

### Protective equipment



### Appropriate engineering controls

Use process enclosures, local exhaust ventilation or other engineering controls as the primary means to minimise worker exposure. Ensure the ventilation system is regularly maintained and tested. In case of insufficient ventilation, wear suitable respiratory equipment. Observe any occupational exposure limits for the product or ingredients.

### Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

### Hand protection

Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacture, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, gloves should comply with European Standard EN374. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.

### Other skin and body protection

Wear appropriate clothing to prevent any possibility of skin contact.

### Hygiene measures

Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.

### Respiratory protection

Ensure all respiratory protective equipment is suitable for its intended use and is 'CE'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

### Environmental exposure controls

Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Appearance	Clear liquid.
Colour	Yellow.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	No information available.
Initial boiling point and range	83 - 85°C/181.4 - 185°F @ 15 mm Hg
Flash point	81°C/177.8°F Closed cup.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.

## 4-(Trifluoromethoxy)aniline

Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	1.32
Solubility(ies)	No information available.
Partition coefficient	No information available.
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

### 9.2. Other information

Molecular weight	177.12
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## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Reactivity	See the other subsections of this section for further details.
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### 10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.
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### 10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	No potentially hazardous reactions known.
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### 10.4. Conditions to avoid

Conditions to avoid	Avoid heat, flames and other sources of ignition.
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### 10.5. Incompatible materials

Materials to avoid	Avoid contact with strong oxidising agents. Strong reducing agents. Strong acids. Strong alkalis.
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### 10.6. Hazardous decomposition products

Hazardous decomposition products	Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO <sub>2</sub> ). Nitrous gases (NO <sub>x</sub> ). Hydrogen fluoride (HF).
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## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

#### Acute toxicity - oral

Summary	Toxic if swallowed.
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Acute toxicity oral (LD <sub>50</sub> mg/kg)	132.0
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Species	Rat
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ATE oral (mg/kg)	132.0
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#### Acute toxicity - dermal

Summary	Fatal in contact with skin.
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## 4-(Trifluoromethoxy)aniline

<b>Acute toxicity dermal (LD<sub>50</sub> mg/kg)</b>	105.0
<b>Species</b>	Rabbit
<b>ATE dermal (mg/kg)</b>	105.0
<b><u>Acute toxicity - inhalation</u></b>	
<b>Summary</b>	Fatal if inhaled.
<b>Acute toxicity inhalation (LC<sub>50</sub> vapours mg/l)</b>	1.0
<b>Species</b>	Rat
<b>ATE inhalation (vapours mg/l)</b>	1.0
<b><u>Skin corrosion/irritation</u></b>	
<b>Summary</b>	Causes skin irritation.
<b><u>Serious eye damage/irritation</u></b>	
<b>Summary</b>	Causes serious eye damage.
<b><u>Respiratory sensitisation</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b><u>Skin sensitisation</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b><u>Germ cell mutagenicity</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b><u>Carcinogenicity</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b>IARC carcinogenicity</b>	None of the ingredients are listed or exempt.
<b><u>Reproductive toxicity</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b><u>Specific target organ toxicity - single exposure</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b><u>Specific target organ toxicity - repeated exposure</u></b>	
<b>Summary</b>	May cause damage to organs through prolonged or repeated exposure.
<b><u>Aspiration hazard</u></b>	
<b>Summary</b>	Based on available data the classification criteria are not met.
<b><u>General information</u></b>	
<b>General information</b>	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
<b>Inhalation</b>	A single exposure may cause the following adverse effects: Difficulty in breathing. Unconsciousness, possibly death.
<b>Ingestion</b>	May cause stomach pain or vomiting. May cause severe internal injury.
<b>Skin contact</b>	A single exposure may cause the following adverse effects: Pain. Unconsciousness, possibly death.

## 4-(Trifluoromethoxy)aniline

<b>Eye contact</b>	Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.
<b>Route of exposure</b>	Ingestion Inhalation Skin and/or eye contact
<b>Target organs</b>	No specific target organs known.

### SECTION 12: Ecological information

#### 12.1. Toxicity

##### Acute aquatic toxicity

**Summary** Based on available data the classification criteria are not met.

##### Chronic aquatic toxicity

**Summary** Harmful to aquatic life with long lasting effects.

#### 12.2. Persistence and degradability

**Persistence and degradability** The degradability of the product is not known.

#### 12.3. Bioaccumulative potential

**Bioaccumulative potential** No data available on bioaccumulation.

**Partition coefficient** No information available.

#### 12.4. Mobility in soil

**Mobility** No data available.

#### 12.5. Results of PBT and vPvB assessment

#### 12.6. Other adverse effects

**Other adverse effects** None known.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

**General information** The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.

**Disposal methods** Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

### SECTION 14: Transport information

**General** For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

#### 14.1. UN number

**UN No. (ADR/RID)** 2810

**UN No. (IMDG)** 2810

**UN No. (ICAO)** 2810



## 4-(Trifluoromethoxy)aniline

UN No. (ADN) 2810

### 14.2. UN proper shipping name

Proper shipping name (ADR/RID) TOXIC LIQUID, ORGANIC, N.O.S. (4-(Trifluoromethoxy)aniline)

Proper shipping name (IMDG) TOXIC LIQUID, ORGANIC, N.O.S. (4-(Trifluoromethoxy)aniline)

Proper shipping name (ICAO) TOXIC LIQUID, ORGANIC, N.O.S. (4-(Trifluoromethoxy)aniline)

Proper shipping name (ADN) TOXIC LIQUID, ORGANIC, N.O.S. (4-(Trifluoromethoxy)aniline)

### 14.3. Transport hazard class(es)

ADR/RID class 6.1

ADR/RID classification code T1

ADR/RID label 6.1

IMDG class 6.1

ICAO class/division 6.1

ADN class 6.1

#### Transport labels



### 14.4. Packing group

ADR/RID packing group II

IMDG packing group II

ICAO packing group II

ADN packing group II

### 14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

### 14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS F-A, S-A

ADR transport category 2

Emergency Action Code 2X

Hazard Identification Number (ADR/RID) 60

Tunnel restriction code (D/E)

### 14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

Annex II of MARPOL 73/78  
and the IBC Code

## 4-(Trifluoromethoxy)aniline

### SECTION 15: Regulatory information

#### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

<b>National regulations</b>	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
<b>EU legislation</b>	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (as amended). Commission Regulation (EU) No 2015/830 of 28 May 2015. Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures (as amended).

#### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

#### Inventories

##### **EU - EINECS/ELINCS**

None of the ingredients are listed or exempt.

### SECTION 16: Other information

<b>Abbreviations and acronyms used in the safety data sheet</b>	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road. ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways. RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail. IATA: International Air Transport Association. ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air. IMDG: International Maritime Dangerous Goods. CAS: Chemical Abstracts Service. ATE: Acute Toxicity Estimate. LC <sub>50</sub> : Lethal Concentration to 50 % of a test population. LD <sub>50</sub> : Lethal Dose to 50% of a test population (Median Lethal Dose). EC <sub>50</sub> : 50% of maximal Effective Concentration. PBT: Persistent, Bioaccumulative and Toxic substance. vPvB: Very Persistent and Very Bioaccumulative.
<b>Classification abbreviations and acronyms</b>	Acute Tox. = Acute toxicity Eye Dam. = Serious eye damage Skin Irrit. = Skin irritation STOT RE = Specific target organ toxicity-repeated exposure Aquatic Chronic = Hazardous to the aquatic environment (chronic)
<b>Classification procedures according to Regulation (EC) 1272/2008</b>	Acute Tox. 2 - H310: Acute Tox. 2 - H330: Acute Tox. 3 - H301: Eye Dam. 1 - H318: STOT RE 2 - H373: Skin Irrit. 2 - H315: : Expert judgement. Aquatic Chronic 3 - H412: : Expert judgement.
<b>Training advice</b>	Only trained personnel should use this material.
<b>Revision date</b>	01/12/2021
<b>Revision</b>	1

## 4-(Trifluoromethoxy)aniline

<b>SDS number</b>	541
<b>Hazard statements in full</b>	H301 Toxic if swallowed. H310 Fatal in contact with skin. H315 Causes skin irritation. H318 Causes serious eye damage. H330 Fatal if inhaled. H373 May cause damage to organs through prolonged or repeated exposure. H412 Harmful to aquatic life with long lasting effects.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.