

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.07.2014

Version 7.1

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

### 1.1 Product identifier

Catalogue No.	818505
Product name	5-Fluorouracil for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	51-21-8

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merck-chemicals.com">www.merck-chemicals.com</a> ).
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### 1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

### 1.4 Emergency telephone number

Please contact the regional company representation in your country.

## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Carcinogenicity, Category 2, H351

Acute toxicity, Category 3, Oral, H301

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

Carc.Cat.3	Carcinogenic Category 3	R40
Xn	Harmful	R22

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word  
Danger

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*Hazard statements*

H301 Toxic if swallowed.  
H351 Suspected of causing cancer.

*Precautionary statements*

Prevention  
P262 Do not get in eyes, on skin, or on clothing.  
P281 Use personal protective equipment as required.  
Response  
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*  
Danger

*Hazard statements*

H301 Toxic if swallowed.  
H351 Suspected of causing cancer.

*Precautionary statements*

P281 Use personal protective equipment as required.  
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 51-21-8

**2.3 Other hazards**

None known.

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**SECTION 3. Composition/information on ingredients**

**3.1 Substance**

Formula C4H3FN2O2 (Hill)  
EC-No. 200-085-6  
Molar mass 130,08 g/mol

**Hazardous components (REGULATION (EC) No 1272/2008)**

*Chemical Name (Concentration)*

CAS-No.	Registration number	Classification
5-fluorouracil (<= 100 % )		
51-21-8	*)	

Acute toxicity, Category 3, H301  
Carcinogenicity, Category 2, H351

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

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**Hazardous components (1999/45/EC)**

*Chemical Name (Concentration)*

CAS-No. Classification

5-fluorouracil ( $\leq 100\%$ )

51-21-8 Carc. Cat. 3; R40  
Xn, Harmful; R22

For the full text of the R-phrases mentioned in this Section, see Section 16.

**3.2 Mixture**

not applicable

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**SECTION 4. First aid measures**

**4.1 Description of first aid measures**

After inhalation: fresh air. Get medical attention.

After skin contact: wash off with plenty of water. Remove contaminated clothing. Get medical attention.

After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophthalmologist if necessary.

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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

irritant effects, Diarrhoea, Nausea, Vomiting, Stomach/intestinal disorders

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

No information available.

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**SECTION 5. Firefighting measures**

**5.1 Extinguishing media**

*Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

*Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

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

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

Hydrogen fluoride, nitrogen oxides

**5.3 Advice for firefighters**

*Special protective equipment for firefighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

*Further information*

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6. Accidental release measures**

**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

**6.2 Environmental precautions**

Do not empty into drains.

**6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

**6.4 Reference to other sections**

Indications about waste treatment see section 13.

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**SECTION 7. Handling and storage**

**7.1 Precautions for safe handling**

*Advice on safe handling*

Work under hood. Do not inhale substance/mixture.

Observe label precautions.

*Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

**7.2 Conditions for safe storage, including any incompatibilities**

*Storage conditions*

Tightly closed. Dry. Keep in a well-ventilated place. Protected from light. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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**SECTION 8. Exposure controls/personal protection**

**8.1 Control parameters**

**8.2 Exposure controls**

**Engineering measures**

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

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**Individual protection measures**

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

*Eye/face protection*

Safety glasses

*Hand protection*

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

*Other protective equipment*

protective clothing

*Respiratory protection*

required when dusts are generated.

Recommended Filter type: Filter P 3 (acc. to DIN 3181) for solid and liquid particles of toxic and very toxic substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

**Environmental exposure controls**

Do not empty into drains.

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**SECTION 9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

Form	powder, finecrystalline
Colour	white
Odour	odourless
Odour Threshold	not applicable

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pH	4,3 - 5,3 at 10 g/l 20 °C
Melting point	282 - 283 °C (decomposition)
Boiling point/boiling range	190 - 200 °C at 0,13 hPa
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Density	No information available.
Relative density	No information available.
Water solubility	12 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: -0,89 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	> 200 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

none

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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

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**10.2 Chemical stability**

heat-sensitive  
Sensitivity to light

**10.3 Possibility of hazardous reactions**

Violent reactions possible with:  
Strong oxidizing agents, Bases

**10.4 Conditions to avoid**

Strong heating (decomposition).

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

in the event of fire: See section 5.

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**SECTION 11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

LD50 rat: 230 mg/kg (RTECS)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

absorption

*Acute inhalation toxicity*

This information is not available.

*Acute dermal toxicity*

absorption

*Skin irritation*

slight irritation

*Eye irritation*

This information is not available.

*Sensitisation*

This information is not available.

*Germ cell mutagenicity*

This information is not available.

*Carcinogenicity*

This information is not available.

*Reproductive toxicity*

This information is not available.

*Teratogenicity*

This information is not available.

*CMR effects*

Carcinogenicity:

Suspected of causing cancer.

*Specific target organ toxicity - single exposure*

This information is not available.

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*Specific target organ toxicity - repeated exposure*

This information is not available.

*Aspiration hazard*

This information is not available.

**11.2 Further information**

Systemic effects:

Nausea, Vomiting, Stomach/intestinal disorders, Diarrhoea, Changes in the blood count

Further data:

Therapeutically used substance.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

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**SECTION 12. Ecological information**

**12.1 Toxicity**

*Toxicity to fish*

LC50 Oncorhynchus mykiss (rainbow trout): > 1.000 mg/l; 48 h (External MSDS)

**12.2 Persistence and degradability**

*Biodegradability*

0 %; 21 d

OECD Test Guideline 301C

Not readily biodegradable.

0 %; 14 d

OECD Test Guideline 302B

Not readily eliminated from water.

**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: -0,89

(experimental)

(Lit.) Bioaccumulation is not expected.

**12.4 Mobility in soil**

No information available.

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

**12.6 Other adverse effects**

*Additional ecological information*

Discharge into the environment must be avoided.



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**SECTION 13. Disposal considerations**

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**SECTION 14. Transport information**

**Land transport (ADR/RID)**

14.1 UN number	UN 2811
14.2 Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (5-FLUORO-2,4-DIHYDROXYPYRIMIDINE)
14.3 Class	6.1
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	E

**Inland waterway transport (ADN)**

Not relevant

**Air transport (IATA)**

14.1 UN number	UN 2811
14.2 Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (5-FLUORO-2,4-DIHYDROXYPYRIMIDINE)
14.3 Class	6.1
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

**Sea transport (IMDG)**

14.1 UN number	UN 2811
14.2 Proper shipping name	TOXIC SOLID, ORGANIC, N.O.S. (5-FLUORO-2,4-DIHYDROXYPYRIMIDINE)
14.3 Class	6.1
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-A S-A

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code  
Not relevant

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**SECTION 15. Regulatory information**

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

*EU regulations*

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Major Accident Hazard Legislation 96/82/EC  
Directive 96/82/EC does not apply

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Take note of Dir 92/85/EEC on the safety and health at work of pregnant workers.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq 0.1\%$  (w/w).

*National legislation*

Storage class 6.1C

## 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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## SECTION 16. Other information

### Full text of H-Statements referred to under sections 2 and 3.

H301 Toxic if swallowed.  
H351 Suspected of causing cancer.


### Full text of R-phrases referred to under sections 2 and 3

R22 Harmful if swallowed.  
R40 Limited evidence of a carcinogenic effect.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling (67/548/EEC or 1999/45/EC)


Symbol(s)	 Xn	Harmful
R-phrases	22-40	Harmful if swallowed. Limited evidence of a carcinogenic effect.
S-phrases	22-24/25-36/37	Do not breathe dust. Avoid contact with skin and eyes. Wear suitable protective clothing and gloves.
EC-No.	200-085-6	

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**Reduced labelling (≤125 ml)**

Symbol(s)  Xn

Harmful

R-phrases 22-40

Harmful if swallowed. Limited evidence of a carcinogenic effect.

S-phrases 36/37

Wear suitable protective clothing and gloves.

**Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

**Regional representation**

This information is given on the authorised Safety Data Sheet for your country.

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*