

Creation Date 31-Jan-2013

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Revision Number 1

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

**Product Description:** 7-Chloro-6-nitroquinazolin-4-ol  
**Cat No.** 450790000; 450790050; 450790250  
**Synonyms** 7-Chloro-6-nitro-3,4-dihydroquinazolin-4-one  
**CAS-No** 53449-14-2  
**Molecular Formula** C8 H4 Cl N3 O3

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

**Recommended Use** Laboratory chemicals  
**Uses advised against** No Information available

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

**Company** Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium  
**E-mail address** begel.sdsdesk@thermofisher.com

**1.4. Emergency telephone number** For information in the US, call: 001-800-ACROS-01  
 For information in Europe, call: +32 14 57 52 11  
  
 Emergency Number, Europe: +32 14 57 52 99  
 Emergency Number, US: 001-201-796-7100  
  
 CHEMTREC Phone Number, US: 001-800-424-9300  
 CHEMTREC Phone Number, Europe: 001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - Regulation (EC) No 1272/2008

##### Physical hazards

Based on available data, the classification criteria are not met

##### Health hazards

Acute oral toxicity	Category 3
Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

##### Environmental hazards

Based on available data, the classification criteria are not met

#### Classification according to EU Directives 67/548/EEC or 1999/45/EC

**Symbol(s)** T - Toxic

**SECTION 2: HAZARDS IDENTIFICATION****R-phrase(s)**

R25 - Toxic if swallowed  
R36/37/38 - Irritating to eyes, respiratory system and skin

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

**2.2. Label elements****Signal Word****Danger****Hazard Statements**

H301 - Toxic if swallowed  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

**Precautionary Statements**

P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

**2.3. Other hazards**

No information available.

**SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008	DSD Classification - 67/548/EEC
7-Chloro-6-nitro-4(3H)-quinazolinone	53449-14-2		>95	Acute Tox. 3 (H301) Eye Irrit. 2 (H319) Skin Irrit. 2 (H315) STOT SE 3 (H335)	T;R25 Xi;R36/37/38

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

**SECTION 4: FIRST AID MEASURES****4.1. Description of first aid measures****Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**Ingestion**

Do not induce vomiting. Call a physician or Poison Control Center immediately.

**Inhalation**

Move to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth resuscitation if victim ingested or inhaled the substance; induce artificial respiration with a respiratory medical device. Immediate medical attention is required.

**Protection of First-aiders**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination

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

No information available

**4.3. Indication of any immediate medical attention and special treatment needed****Notes to Physician**

Treat symptomatically

**SECTION 5: FIREFIGHTING MEASURES****5.1. Extinguishing media****Suitable Extinguishing Media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Extinguishing media which must not be used for safety reasons**

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors

**Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Hydrogen chloride .

**5.3. Advice for firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

**SECTION 6: ACCIDENTAL RELEASE MEASURES****6.1. Personal precautions, protective equipment and emergency procedures**

Ensure adequate ventilation. Use personal protective equipment. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Avoid dust formation.

**6.2. Environmental precautions**

Should not be released into the environment.

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

Sweep up or vacuum up spillage and collect in suitable container for disposal. Avoid dust formation.

**6.4. Reference to other sections**

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7: HANDLING AND STORAGE****7.1. Precautions for safe handling**

Use only under a chemical fume hood. Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Do not breathe vapors/dust. Do not ingest.

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

Keep containers tightly closed in a dry, cool and well-ventilated place.

**7.3. Specific end use(s)**

Use in laboratories

**SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION****8.1. Control parameters****Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

**Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies.

**Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

**Derived No Effect Level (DNEL)** No information available.

Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral Dermal Inhalation				

**Predicted No Effect Concentration (PNEC)** No information available.

**8.2. Exposure controls****Engineering Measures**

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Wear natural rubber gloves Nitrile rubber Neoprene PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. Remove gloves with care avoiding skin contamination.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

<b>Respiratory Protection</b>	When workers are facing concentrations above the exposure limit they must use appropriate certified respirators To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly.
<b>Large scale/emergency use</b>	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. <b>Recommended Filter type:</b> Particulates filter conforming to EN 143
<b>Small scale/Laboratory use</b>	Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. <b>Recommended half mask:-</b> Particle filtering: EN149:2001 When RPE is used a face piece Fit Test should be conducted.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice
<b>Environmental exposure controls</b>	No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

<b>Appearance</b>		
<b>Physical State</b>	Solid.	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No data available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No data available	
<b>Flash Point</b>	No information available.	<b>Method -</b> No information available.
<b>Evaporation Rate</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available.	
<b>Explosion Limits</b>	No data available.	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	No information available.	
<b>Solubility in other solvents</b>	No information available.	
<b>Partition Coefficient (n-octanol/water)</b>	<b>Component</b> 7-Chloro-6-nitro-4(3H)-quinazolinone	<b>log Pow</b> 0,449
<b>Autoignition Temperature</b>	Not applicable	
<b>Decomposition temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Explosive Properties</b>	No information available.	
<b>Oxidizing Properties</b>	No information available.	

### 9.2. Other information

<b>Molecular Formula</b>	C8 H4 Cl N3 O3
<b>Molecular Weight</b>	225.59

**SECTION 10: STABILITY AND REACTIVITY****10.1. Reactivity**

None known, based on information available.

**10.2. Chemical stability**

Stable under normal conditions.

**10.3. Possibility of hazardous reactions****Hazardous Polymerization**

No information available

**Hazardous Reactions**

None under normal processing..

**10.4. Conditions to avoid**

Incompatible products, Excess heat, Avoid dust formation, Exposure to moisture.

**10.5. Incompatible materials**

Strong oxidizing agents. Acids. Bases.

**10.6. Hazardous decomposition products**Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Hydrogen chloride .**SECTION 11: TOXICOLOGICAL INFORMATION****11.1. Information on toxicological effects****Product Information****(a) acute toxicity;****Oral**

Category 3

**Dermal**

No data available

**Inhalation**

No data available

**(b) skin corrosion/irritation;**

Category 2

**(c) serious eye damage/irritation;**

Category 2

**(d) respiratory or skin sensitization;****Respiratory**

No data available

**Skin**

No data available

**(e) germ cell mutagenicity;**

No data available

**(f) carcinogenicity;**

No data available

There are no known carcinogenic chemicals in this product

**(g) reproductive toxicity;**

No data available

**(h) STOT-single exposure;**

Category 3

**(i) STOT-repeated exposure;**

No data available

**Target Organs**

None known.

**(j) aspiration hazard;**

Not applicable

Solid

**Other Adverse Effects**

The toxicological properties have not been fully investigated.

Symptoms / effects,  
both acute and delayed

No information available.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

Ecotoxicity effects

Do not empty into drains.

12.2. Persistence and degradability

No information available

12.3. Bioaccumulative potential

No information available.

Component	log Pow	Bioconcentration factor (BCF)
7-Chloro-6-nitro-4(3H)-quinazolinone	0,449	No data available

12.4. Mobility in soil

No information available.

12.5. Results of PBT and vPvB  
assessment

No data available for assessment

### 12.6. Other adverse effects

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

Persistent Organic Pollutant

This product does not contain any known or suspected substance

Ozone Depletion Potential

This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

Waste from Residues / Unused  
Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. .

European Waste Catalogue (EWC)

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

14.1. UN number

UN2811

14.2. UN proper shipping name

Toxic solid, organic, n.o.s

14.3. Transport hazard class(es)

6.1

14.4. Packing group

III

### ADR

14.1. UN number

UN2811

14.2. UN proper shipping name

Toxic solid, organic, n.o.s

14.3. Transport hazard class(es)

6.1

14.4. Packing group

III

### IATA

14.1. UN number

UN2811

14.2. UN proper shipping name

Toxic solid, organic, n.o.s

14.3. Transport hazard class(es)

6.1

14.4. Packing group

III

<b>14.5. Environmental hazards</b>	No hazards identified
<b>14.6. Special precautions for user</b>	No special precautions required
<b>14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

**International Inventories** X = listed

#### National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment  
Take note of Dir 94/33/EC on the protection of young people at work

### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

R25 - Toxic if swallowed  
R36/37/38 - Irritating to eyes, respiratory system and skin

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

H301 - Toxic if swallowed  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

### Legend

**CAS** - Chemical Abstracts Service  
**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances  
**PICCS** - Philippines Inventory of Chemicals and Chemical Substances  
**IECSC** - China Inventory of Existing Chemical Substances  
**KECL** - Existing and Evaluated Chemical Substances

**WEL** - Workplace Exposure Limit  
**ACGIH** - American Conference of Industrial Hygiene  
**DNEL** - Derived No Effect Level  
**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory  
**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List  
**ENCS** - Japan Existing and New Chemical Substances  
**AICS** - Australian Inventory of Chemical Substances  
**NZIoC** - New Zealand Inventory of Chemicals

**TWA** - Time Weighted Average  
**IARC** - International Agency for Research on Cancer  
**PNEC** - Predicted No Effect Concentration  
**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association  
**MARPOL** - International Convention for the Prevention of Pollution from Ships  
**ATE** - Acute Toxicity Estimate  
**VOC** - Volatile Organic Compounds



**Key literature references and sources for data**

Suppliers safety data sheet,  
Chemadvisor - LOLI,  
Merck index,  
RTECS

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Creation Date** 31-Jan-2013

**Revision Date** 31-Jan-2013

**Revision Summary**

**Reason for revision** Not applicable

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006**

**Disclaimer**

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

**End of Safety Data Sheet**