

Revision Date 03-Dec-2013

Revision Number 4

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

1.1. Product identifier

Product Description: **3-(tert-Butyl)-1-methyl-1H-pyrazole-carboxylic acid, 95%**
 Cat No. : **452620000; 452620050; 452620500**
 CAS-No **175277-11-9**
 Molecular Formula **C9 H14 N2 O2**

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 begeel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **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

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)	Xi - Irritant
R-phrases(s)	none
	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****Warning****Hazard Statements**

H315 - Causes skin irritation
 H335 - May cause respiratory irritation
 H319 - Causes serious eye irritation

Precautionary Statements

P261 - Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray
 P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
 P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection
 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
3-(tert-Butyl)-1-methyl-1H-pyrazole-5-carboxylic acid	175277-11-9		>=95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)	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. Obtain medical attention.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention if symptoms occur..

Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Inhalation

Move to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Get medical attention immediately if symptoms occur.

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

Water spray. Carbon dioxide (CO₂). Dry chemical. chemical foam.

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

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂).

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.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so

6.3. Methods and material for containment and cleaning up

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

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

Ensure adequate ventilation. Wear personal protective equipment. Avoid contact with skin, eyes and clothing. Avoid ingestion and inhalation. Wash hands before breaks and immediately after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

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

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

3-(tert-Butyl)-1-methyl-1H-pyrazole-carboxylic acid, 95%**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.

<u>Route of exposure</u>	<u>Acute effects (local)</u>	<u>Acute effects (systemic)</u>	<u>Chronic effects (local)</u>	<u>Chronic effects (systemic)</u>
Oral Dermal Inhalation				

Predicted No Effect Concentration (PNEC) No information available.

8.2. Exposure controls**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. 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

<u>Glove material</u>	<u>Breakthrough time</u>	<u>Glove thickness</u>	<u>EU standard</u>	<u>Glove comments</u>
Natural rubber Butyl rubber 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

Respiratory Protection No protective equipment is needed under normal use conditions.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced..

Small scale/Laboratory use Maintain adequate ventilation

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance	Off-white	
Physical State	Solid.	
Odor	No information available	
Odor Threshold	No data available	
pH	No data available	
Melting Point/Range	151 - 154°C / 303.8 - 309.2°F	Measured
Softening Point	No data available	
Boiling Point/Range	No information available.	
Flash Point	No information available.	Method - No information available.
Evaporation Rate	Not applicable	Solid
Flammability (solid,gas)	No information available.	
Explosion Limits	No data available.	
Vapor Pressure	No data available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	No information available.	
Solubility in other solvents	No information available.	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	Not applicable	
Decomposition temperature	No data available	
Viscosity	Not applicable	Solid
Explosive Properties	No information available.	
Oxidizing Properties	No information available.	

9.2. Other information

Molecular Formula C9 H14 N2 O2
Molecular Weight 182.22

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 No information available.

10.4. Conditions to avoid

Incompatible products, Excess heat, Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents. Bases. Reducing agents.

10.6. Hazardous decomposition productsNitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂).**SECTION 11: TOXICOLOGICAL INFORMATION****11.1. Information on toxicological effects****Product Information**

No acute toxicity information is available for this product

(a) acute toxicity;

Oral

No data available

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

No information available.

(j) aspiration hazard;

Not applicable

Solid

Other Adverse Effects**Symptoms / effects,
both acute and delayed**

The toxicological properties have not been fully investigated.

No information available.

SECTION 12: ECOLOGICAL INFORMATION**12.1. Toxicity****Ecotoxicity effects**

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants

12.2. Persistence and degradability

No information available

12.3. Bioaccumulative potential

No information 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	Not regulated
14.1. UN number	
14.2. UN proper shipping name	
14.3. Transport hazard class(es)	
14.4. Packing group	
ADR	Not regulated
14.1. UN number	
14.2. UN proper shipping name	
14.3. Transport hazard class(es)	
14.4. Packing group	
IATA	Not regulated
14.1. UN number	
14.2. UN proper shipping name	
14.3. Transport hazard class(es)	
14.4. Packing group	
14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required
14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	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
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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

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents 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**

R36/37/38 - Irritating to eyes, respiratory system and skin

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

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.

Revision Date

03-Dec-2013

Revision Summary

Reason for revision

(M)SDS sections updated, 4, 7, 8, 10, 11, 12, 13.

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