

Creation Date 20-Oct-2010

Revision Date 05-Dec-2014

Revision Number 2

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

1.1. Product identification

Product Description: Cat No. : CAS-No Molecular Formula	<u>4-Bromo-3-(trifluoromethyl)-1H-pyrazole</u> 438040000; 438040010; 438040050 19968-17-3 C4 H2 Br F3 N2
1.2. Relevant identified uses of th	e substance or mixture and uses advised against
Recommended Use Uses advised against	Laboratory chemicals. No Information available
1.3. Details of the supplier of the	safety data sheet
Company	Acros Organics BVBA Janssen Pharmaceuticalaan 3a 2440 Geel, Belgium

begel.sdsdesk@thermofisher.com

E-mail address

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

Physical hazards Based on available data, the classification criteria are not met		
Health hazards		
Acute oral toxicity	Category 4	
Acute dermal toxicity	Category 4	
Acute Inhalation Toxicity - Dusts and Mists	Category 4	
Skin Corrosion/irritation	Category 2	
Serious Eye Damage/Eye Irritation	Category 2	
Specific target organ toxicity - (single exposure)	Category 3	

Classification accordin	ng to EU Directives 67/548/EEC or 1999/45/EC
Symbol(s)	Xn - Harmful
R-phrase(s)	
,	R20/21/22 - Harmful by inhalation in conta

armful by inhalation, in contact with skin and if swallowed R36/37/38 - Irritating to eyes, respiratory system and skin

4-Bromo-3-(trifluoromethyl)-1H-pyrazole

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

- H302 Harmful if swallowed
- H312 Harmful in contact with skin
- H315 Causes skin irritation
- H319 Causes serious eye irritation
- H332 Harmful if inhaled
- H335 May cause respiratory irritation

Precautionary Statements

P280 - Wear protective gloves/ eye protection/ face protection

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P304 + P341 - IF INHALED: If breathing is difficult, remove to fresh air and keep at rest in a position comfortable for breathing P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P312 - Call a POISON CENTER or doctor/ physician if you feel unwell

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
4-Bromo-3-(trifluoromethyl)-1H-pyra zole	19968-17-3		>95	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)	Xn;R20/21/22 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 plenty of water for at least 15 minutes. 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. 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

4-Bromo-3-(trifluoromethyl)-1H-pyrazole

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 (CO₂), Nitrogen oxides (NOx), Hydrogen fluoride.

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. Avoid dust formation.

6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional ecological information.

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

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Use only under a chemical fume hood. Wear personal protective equipment. Do not get in eyes, on skin, or on 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 container tightly closed in a dry and well-ventilated place. To maintain product quality. Store under an inert atmosphere.

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 No information available. **(PNEC)**

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	Prote	ctive gloves		
Glove material Natural rubber Nitrile rubber Neoprene PVC	Breakthrough time See manufacturers recommendations	Glove thickness -	EU standard EN 374	Glove comments (minimum requirement)
Skin and body pr	rotection Wear	appropriate protectiv	ve gloves and clothing to	o prevent skin exposure
(Refer to manufacture Ensure gloves are suit sensitisation effects, a of cuts, abrasion.	structions regarding per r/supplier for informatio table for the task: Chen	n) nical compatability, E ion the specific loca	Dexterity, Operational co	provided by the supplier of the gloves. Inditions, User susceptibility, e.g. In the product is used, such as the danger
Respiratory Prote	appro To pro	priate certified respire	rators.	e exposure limit they must use oment must be the correct fit and be used
	appro To pro and m ncy use Use a are ex	priate certified respin otect the wearer, res aaintained properly NIOSH/MSHA or El acceeded or if irritation	rators. piratory protective equip	oment must be the correct fit and be used 36 approved respirator if exposure limits e experienced
Respiratory Prote	appro To pro and m acy use Use a are ex Reco Dry use Use a limits Reco 141	priate certified respin betect the wearer, res aaintained properly NIOSH/MSHA or El ceeded or if irritation mmended Filter typ NIOSH/MSHA or El are exceeded or if ir mmended half mas	rators. piratory protective equip uropean Standard EN 1 n or other symptoms are be: Particulates filter co uropean Standard EN 1 ritation or other symptor	oment must be the correct fit and be used 36 approved respirator if exposure limits e experienced nforming to EN 143 49:2001 approved respirator if exposure ns are experienced. 05; or; Half mask: EN140; plus filter, EN
Large scale/emergen	appro To pro and m are ex Reco Dry use Use a limits Reco 141 When	priate certified respin betect the wearer, res naintained properly NIOSH/MSHA or El ceeded or if irritation mmended Filter typ NIOSH/MSHA or El are exceeded or if ir mmended half mas RPE is used a face	rators. piratory protective equip uropean Standard EN 1 n or other symptoms are be: Particulates filter co uropean Standard EN 1 ritation or other symptor k:- Valve filtering: EN4	oment must be the correct fit and be used 36 approved respirator if exposure limits e experienced nforming to EN 143 49:2001 approved respirator if exposure ns are experienced. 05; or; Half mask: EN140; plus filter, EN e conducted

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

4-Bromo-3-(trifluoromethyl)-1H-pyrazole

Appearance Physical State	White Solid	
Odor Odor Threshold pH Melting Point/Range Softening Point Boiling Point/Range Flash Point Evaporation Rate Flammability (solid,gas) Explosion Limits	No information available No data available No information available 112 - 114 °C / 233.6 - 237.2 °F No data available No information available No data available Not applicable No information available No data available	Measured Method - No information available Solid
Vapor Pressure Vapor Density Specific Gravity / Density Bulk Density Water Solubility Solubility in other solvents	No data available Not applicable No data available No data available No information available No information available	Solid

4-Bromo-3-(trifluoromethyl)-1H-pyrazole

Partition Coefficient (n-octanol/wat	er)	
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 Molecular Weight	C4 H2 Br F3 N2 214.97	

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 Hazardous Reactions	Hazardous polymerization does not occur. None under normal processing.
10.4. Conditions to avoid	Incompatible products. Excess heat. Avoid dust formation.
10.5. Incompatible materials	

Strong oxidizing agents. Strong acids. Strong bases.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NOx). Hydrogen fluoride.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on toxicological effects

Product Information

Category 4 Category 4 Category 4
Category 2
Category 2
No data available No data available
No data available
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	Eyes, Skin, Respiratory system.
(j) aspiration hazard;	Not applicable Solid

Symptoms / effects,both acute and No information available delayed

SECTION 12: ECOLOGICAL INFORMATION

<u>12.1. Toxicity</u> 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	
<u>12.4. Mobility in soil</u> <u>12.5. Results of PBT and vPvB</u>	No information available No data available for assessment.	
assessment		
12.6. Other adverse effects Endocrine Disruptor Information Persistent Organic Pollutant Ozone Depletion Potential	This product does not contain any known or suspected endocrine disruptors This product does not contain any known or suspected substance This product does not contain any known or suspected substance	
SECTION 13: DISPOSAL CONSIDERATIONS		

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

ACR43804

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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 Not applicable, packaged goods Annex II of MARPOL73/78 and the IBC Code	

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 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

R20/21/22 - Harmful by inhalation, in contact with skin and if swallowed R36/37/38 - Irritating to eyes, respiratory system and skin

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

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H332 - Harmful if inhaled

H335 - May cause respiratory irritation

Legend

4-Bromo-3-(trifluoromethyl)-1H-pyrazole

CAS - Chemical Abstracts Service	TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
EINECS/ELINCS - European Inventory of Existing Commercial Chemica	I DSL/NDSL - Canadian Domestic Substances List/Non-Domestic
Substances/EU List of Notified Chemical Substances	Substances List
PICCS - Philippines Inventory of Chemicals and Chemical Substances	ENCS - Japanese Existing and New Chemical Substances
IECSC - Chinese Inventory of Existing Chemical Substances	AICS - Australian Inventory of Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances	NZIOC - New Zealand Inventory of Chemicals
WEL - Workplace Exposure Limit	TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	PNEC - Predicted No Effect Concentration
RPE - Respiratory Protective Equipment	LD50 - Lethal Dose 50%
LC50 - Lethal Concentration 50%	EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration	POW - Partition coefficient Octanol:Water
PBT - Persistent, Bioaccumulative, Toxic	vPvB - very Persistent, very Bioaccumulative
ADR - European Agreement Concerning the International Carriage of	ICAO/IATA - International Civil Aviation Organization/International Air
Dangerous Goods by Road	Transport Association
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code	MARPOL - International Convention for the Prevention of Pollution from Ships
OECD - Organisation for Economic Co-operation and Development	ATE - Acute Toxicity Estimate
BCF - Bioconcentration factor	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.

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Revision Summary	Update to Format, (M)SDS sections updated, 2, 4, 5, 7, 8, 9, 10, 11.

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