

Safety Data Sheet

according to UK REACH Regulation

QNB

Revision date: 27.04.2022

Product code: 2830

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

QNB

Further trade names

Benzeneacetic acid, a-hydroxy-a-phenyl-, 1-azabicyclo[2.2.2]oct-3-yl ester

Synonyms:3-Quinuclidinol, benzilate (ester); Benzilic acid, 3-quinuclidinyl ester; β -Quinuclidinyl benzilate;
3-Hydroxyquinuclidine benzilate; 3-Oxyquinuclidine benzilate; 3-Quinuclidinol benzilate; 3-Quinuclidinyl
benzilate; 3-Quinuclidyl benzilate; NSC 173698; Ro 2-3308

CAS No: 6581-06-2

1.2. Relevant identified uses of the substance or mixture and uses advised against**Use of the substance/mixture**Precursor for [^{11}C]Me-QNB
([^{11}C]N-methyl-quinuclidin-3-yl benzilate)**1.3. Details of the supplier of the safety data sheet**

Company name:	ABX advanced biochemical compounds	
	Biomedizinische Forschungsreagenzien GmbH	
Street:	Heinrich-Gläser-Straße 10-14	
Place:	01454 Radeberg	
Telephone:	+49 3528 4041 60	Telefax: +49 3528 4041 65
e-mail:	info@abx.de	
Contact person:	Dr. Christoph Meyer	Telephone: +49 3528 4041 8732
e-mail:	meyer@abx.de	
Internet:	http://www.abx.de	

1.4. Emergency telephone number:

+49 3528 4041 60

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****GB CLP Regulation**

Acute Tox. 2; H300

Full text of hazard statements: see SECTION 16.

2.2. Label elements**GB CLP Regulation****Hazard components for labelling**

3-Quinuclidinyl benzilate

Signal word: Danger**Pictograms:****Hazard statements**

H300	Fatal if swallowed.
H300+H330	Fatal if swallowed or if inhaled.

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Precautionary statements

- P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
- P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.

SECTION 3: Composition/information on ingredients**3.1. Substances****Chemical characterization**

Benzeneacetic acid, a-hydroxy-a-phenyl-, 1-azabicyclo[2.2.2]oct-3-yl ester

Sum formula: C₂₁H₂₃NO₃

Molecular weight: 337.41

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
6581-06-2	3-Quinuclidinyl benzilate			95 - < 100 %
	Acute Tox. 2; H300			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
6581-06-2		3-Quinuclidinyl benzilate	95 - < 100 %
		oral: LD50 = 8 - 14 mg/kg	

SECTION 4: First aid measures**4.1. Description of first aid measures****After inhalation**

Provide fresh air.

After contact with skin

After contact with skin, wash immediately with: Water. Change contaminated clothing.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

If swallowed, immediately drink: Water. Call a physician immediately.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**Co-ordinate fire-fighting measures to the fire surroundings. Suitable extinguishing media: Foam. Extinguishing powder. Carbon dioxide (CO₂). Atomized water.**5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.

Additional information

Contaminated fire-fighting water must be collected separately. Do not allow to enter into surface water or drains.

SECTION 6: Accidental release measures

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6.2. Environmental precautions

Do not allow to enter into surface water or drains.

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

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

Do not breathe dust. Conditions to avoid: skin contact. Eye contact. Wear personal protection equipment.
When using do not eat, drink, smoke, sniff.

Advice on general occupational hygiene

Change contaminated clothing. Wash hands before breaks and after work. When using do not eat or drink.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container dry. Keep container tightly closed.

Further information on storage conditions

Recommended storage temperature:

of °C: 2

up to °C: 8

Protect against: Light. Store under (Gas): argon. Nitrogen.

SECTION 8: Exposure controls/personal protection**8.1. Control parameters****Additional advice on limit values**

To date, no national critical limit values exist.

8.2. Exposure controls**Appropriate engineering controls**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust.

SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state: solid
Colour: colourless

Changes in the physical state

Melting point/freezing point: 163 - 168 °C

Water solubility: partially soluble

Solubility in other solvents

Chloroform. Ethanol dimethylsulphoxide (DMSO).

SECTION 10: Stability and reactivity**10.4. Conditions to avoid**

Light.

10.6. Hazardous decomposition productsCarbon dioxide. Carbon monoxide. Nitrogen oxides (NO_x).

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SECTION 11: Toxicological information**11.1. Information on hazard classes as defined in GB CLP Regulation****Acute toxicity**

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
6581-06-2	3-Quinuclidinyl benzilate				
	oral	LD50 mg/kg	8 - 14	Practical experience/human experience.	

SECTION 12: Ecological information**12.5. Results of PBT and vPvB assessment**

This substance does not meet the PBT/vPvB criteria of UK REACH.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Do not allow to enter into surface water or drains. Dispose of waste according to applicable legislation.

List of Wastes Code - residues/unused products

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

List of Wastes Code - used product

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

List of Wastes Code - contaminated packaging

150110 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); packaging containing residues of or contaminated by hazardous substances; hazardous waste

SECTION 14: Transport information**Land transport (ADR/RID)****14.1. UN number or ID number:**

UN 2811

14.2. UN proper shipping name:

toxic solid, organic, n.o.s. (3-Quinuclidinyl benzilate)

14.3. Transport hazard class(es):

6.1

14.4. Packing group:

II

Hazard label:

6.1

Inland waterways transport (ADN)**14.1. UN number or ID number:**

UN 2811

14.2. UN proper shipping name:

toxic solid, organic, n.o.s. (3-Quinuclidinyl benzilate)

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14.3. Transport hazard class(es):

6.1

14.4. Packing group:

II

Hazard label:

6.1

Marine transport (IMDG)**14.1. UN number or ID number:**

UN 2811

14.2. UN proper shipping name:

toxic solid, organic, n.o.s. (3-Quinuclidinyl benzilate)

14.3. Transport hazard class(es):

6.1

14.4. Packing group:

II

Hazard label:

6.1

Air transport (ICAO-TI/IATA-DGR)**14.1. UN number or ID number:**

UN 2811

14.2. UN proper shipping name:

toxic solid, organic, n.o.s. (3-Quinuclidinyl benzilate)

14.3. Transport hazard class(es):

6.1

14.4. Packing group:

II

Hazard label:

6.1

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****National regulatory information**

Water hazard class (D):

3 - highly hazardous to water

SECTION 16: Other information**Relevant H and EUH statements (number and full text)**

H300

Fatal if swallowed.

H300+H330

Fatal if swallowed or if inhaled.