



BENZOIC ACID CALIBRANT FOR QNMR 5mM BENZOIC ACID IN DMSO-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 19/09/2014

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Version: 2.0

DLM-9491

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form	: Mixtures
Product name.	: BENZOIC ACID CALIBRANT FOR QNMR 5mM BENZOIC ACID IN DMSO-D6
Product code	: DLM-9491
Other means of identification	: Also applicable to: DLM-9491A (50UL FILL VOLUME) DLM-9491B (160UL FILL VOLUME) DLM-9491C (750UL FILL VOLUME) DLM-9491D DLM-9491E (120 UL FILL VOLUME)

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

1.2.1. Relevant identified uses

Main use category	: Professional use
Industrial/Professional use spec	: For professional use only.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810
USA

USA: 1-800-322-1174 Int: 1-978-749-8000
cilsales@isotope.com www.isotope.com

Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)
International: 1-703-741-5970 (24 hours)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Skin Irrit. 2 H315
Eye Dam. 1 H318
STOT SE 3 H335

Full text of H-phrases: see section 16

Classification according to Directive 67/548/EEC or 1999/45/EC

Xi; R37/38
Xi; R41
Xn; R22

Full text of R-phrases: see section 16

Classification (GHS-US)

Flam. Liq. 4 H227
Skin Irrit. 2 H315
Eye Dam. 1 H318
STOT SE 3 H335

Adverse physicochemical, human health and environmental effects

Eyes, Skin.

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2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS05

GHS07

Signal word (CLP) :

Danger

Hazard statements (CLP) :

H315 - Causes skin irritation
H318 - Causes serious eye damage
H335 - May cause respiratory irritation

Precautionary statements (CLP) :

P261 - Avoid breathing dust, fume, gas, mist, spray, vapors
P264 - Wash Both hands thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P280 - Wear eye protection, face protection, protective clothing, protective gloves
P302+P352 - IF ON SKIN: Wash with plenty of water/...
P304+P340 - IF INHALED: Remove person to fresh air and keep 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
P310 - Immediately call a POISON CENTER/doctor/...

GHS-US labeling

Hazard pictograms (GHS-US) :



GHS05

GHS07

Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H227 - Combustible liquid
H315 - Causes skin irritation
H318 - Causes serious eye damage
H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors
P264 - Wash Both hands thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P280 - Wear eye protection, face protection, protective clothing, protective gloves
P302+P352 - IF ON SKIN: Wash with plenty of soap and water
P304+P340 - IF INHALED: Remove victim 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
P310 - Immediately call a POISON CENTER or doctor/physician
P312 - Call a POISON CENTER/doctor/physician if you feel unwell
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)
P332+P313 - If skin irritation occurs: Get medical advice/attention
P362 - Take off contaminated clothing and wash before reuse
P370+P378 - In case of fire: Use Alcohol resistant foam., Carbon dioxide., Dry chemical., Water spray for extinction
P403+P233 - Store in a well-ventilated place. Keep container tightly closed
P403+P235 - Store in a well-ventilated place. Keep cool
P405 - Store locked up
P501 - Dispose of contents/container to Comply with applicable regulations.

2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Not applicable

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3.2. Mixtures

Name	Product identifier	%	Classification according to Directive 67/548/EEC
DIMETHYL SULFOXIDE-D6 (D, 99.9%)	(CAS No) 2206-27-1 (EC no) 218-617-0	99.948	Not classified
BENZOIC ACID UNLABELED	(CAS No) 65-85-0 (EC no) 200-618-2	0.052	Xn; R22 Xi; R41 Xi; R37

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
DIMETHYL SULFOXIDE-D6 (D, 99.9%)	(CAS No) 2206-27-1 (EC no) 218-617-0	99.948	Not classified
BENZOIC ACID UNLABELED	(CAS No) 65-85-0 (EC no) 200-618-2	0.052	Acute Tox. 4 (Oral), H302 Eye Dam. 1, H318 STOT SE 3, H335

Full text of R-, H- and EUH-phrases: see section 16

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
First-aid measures after inhalation	: Remove to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER/doctor/physician if you feel unwell.
First-aid measures after skin contact	: Wash with plenty of soap and water. Wash contaminated clothing before reuse. Get medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER or doctor/physician.
First-aid measures after ingestion	: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

Symptoms/injuries after inhalation	: May cause respiratory irritation.
Symptoms/injuries after skin contact	: Causes skin irritation.
Symptoms/injuries after eye contact	: Causes serious eye damage.
Symptoms/injuries after ingestion	: May be harmful if swallowed.

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

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

5.2. Special hazards arising from the substance or mixture

No additional information available

5.3. Advice for firefighters

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Avoid breathing vapors, mist, or gas.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3. Methods and material for containment and cleaning up

For containment : Keep in suitable, closed containers for disposal.

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6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Use only outdoors or in a well-ventilated area.
Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store at room temperature away from light and moisture.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Personal protective equipment : Gloves. Safety glasses. Respiratory protection of the dependent type. Protective clothing.



Hand protection : Wear suitable protective clothing and gloves.
Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.
Skin and body protection : Wear suitable protective clothing.
Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

The properties listed below are for the solvent, the main component of this mixture.

Physical state : Liquid
Appearance : Liquid, clear.
Molecular mass : 84.17 g/mol (Labeled)
Color : Colourless.
Odor : No data available
Odor threshold : No data available
pH : No data available
Relative evaporation rate (butyl acetate=1) : No data available
Melting point : 18.4 °C (65.1 °F)
Freezing point : No data available
Boiling point : 189 °C (372 °F) at 1,013 hPa (760 mmHg)
Flash point : 87 °C (189 °F) - closed cup
Self ignition temperature : 301 °C (574 °F)
Decomposition temperature : No data available
Flammability (solid, gas) : No data available
Vapor pressure : 0.55 hPa (0.41 mmHg) at 20 °C (68 °F)
Relative vapor density at 20 °C : No data available
Relative density : No data available
Density : 1.19 g/ml (Labeled)
Solubility : Water: Completely miscible
Log Pow : No data available
Log Kow : No data available
Viscosity, kinematic : No data available
Viscosity, dynamic : No data available
Explosive properties : No data available

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Oxidizing properties : No data available
Explosive limits : 3.5 - 42 % (V)

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

No additional information available

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

No additional information available

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

BENZOIC ACID CALIBRANT FOR QNMR 5mM BENZOIC ACID IN DMSO-D6	
LD50 oral rat	14500 mg/kg
LD50 dermal rabbit	> 5000 mg/kg
LC50 inhalation rat (ppm)	40250 ppm 4h
ATE (oral)	14500.000 mg/kg body weight

DIMETHYL SULFOXIDE-D6 (D, 99.9%) (2206-27-1)	
LD50 oral rat	14500 mg/kg
LD50 dermal rabbit	> 5000 mg/kg
LC50 inhalation rat (ppm)	40250 ppm 4h
ATE (oral)	14500.000 mg/kg body weight

BENZOIC ACID UNLABELED (65-85-0)	
LD50 oral rat	1700 mg/kg
LD50 dermal rabbit	10000 mg/kg
LC50 inhalation rat (mg/l)	> 12.2 mg/l 4 h
ATE (oral)	1700.000 mg/kg body weight
ATE (dermal)	10000.000 mg/kg body weight

Skin corrosion/irritation : Causes skin irritation.
Skin - rabbit - Mild skin irritation - 24 h

Serious eye damage/irritation : Causes serious eye damage.
Eyes - rabbit - Mild eye irritation

Respiratory or skin sensitization : Not available
No data available

Germ cell mutagenicity : Not available

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

Specific target organ toxicity (single exposure) : May cause respiratory irritation.

Specific target organ toxicity (repeated exposure) : Not classified

Aspiration hazard : Not classified

Symptoms/injuries after inhalation : May cause respiratory irritation.

Symptoms/injuries after skin contact : Causes skin irritation.

Symptoms/injuries after eye contact : Causes serious eye damage.

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Symptoms/injuries after ingestion : May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

BENZOIC ACID CALIBRANT FOR QNMR 5mM BENZOIC ACID IN DMSO-D6	
LC50 fish 1	34000 mg/l Pimephales promelas (fathead minnow) -96h
EC50 Daphnia 1	27500 mg/l Daphnia pulex (Water flea)
ErC50 (algae)	400000 mg/l Lepomis macrochirus (Bluegill) -96h
DIMETHYL SULFOXIDE-D6 (D, 99.9%) (2206-27-1)	
LC50 fish 1	34000 mg/l Pimephales promelas (fathead minnow) - 96h
EC50 Daphnia 1	24600 mg/l Daphnia magna (Water flea) - 48 h
LC50 fish 2	35000 mg/l Oncorhynchus mykiss (rainbow trout) - 96 h
LC50 other aquatic organisms 2	17000 mg/l Pseudokirchneriella subcapitata (green algae) - 72 h
ErC50 (algae)	400000 mg/l Lepomis macrochirus (Bluegill) -96h
BENZOIC ACID UNLABELED (65-85-0)	
LC50 fish 1	180 mg/l Gambusia affinis (Mosquito fish) - 96 h

12.2. Persistence and degradability

BENZOIC ACID CALIBRANT FOR QNMR 5mM BENZOIC ACID IN DMSO-D6	
Persistence and degradability	Not available.
DIMETHYL SULFOXIDE-D6 (D, 99.9%) (2206-27-1)	
Persistence and degradability	Not available.
BOD (% of ThOD)	31 % ThOD
BENZOIC ACID UNLABELED (65-85-0)	
Persistence and degradability	Not available.

12.3. Bioaccumulative potential

DIMETHYL SULFOXIDE-D6 (D, 99.9%) (2206-27-1)	
Log Pow	-1.349
BENZOIC ACID UNLABELED (65-85-0)	
Bioconcentration factor (BCF REACH)	5.3
Bioaccumulative potential	Bioaccumulation: Leuciscus idus (Golden orfe) - 3 d.

12.4. Mobility in soil

BENZOIC ACID UNLABELED (65-85-0)	
Ecology - soil	Not available.

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : Not available.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.

SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

14.1. UN number

UN-No.(DOT) : 1993
DOT NA no. UN1993

14.2. UN proper shipping name

DOT Proper Shipping Name : Flammable liquids, n.o.s.

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Department of Transportation (DOT) Hazard Classes : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
Hazard labels (DOT) : 3 - Flammable liquid



DOT Symbols : G - Identifies PSN requiring a technical name
Packing group (DOT) : III - Minor Danger
DOT Special Provisions (49 CFR 172.102) : B1 - If the material has a flash point at or above 38 C (100 F) and below 93 C (200 F), then the bulk packaging requirements of 173.241 of this subchapter are applicable. If the material has a flash point of less than 38 C (100 F), then the bulk packaging requirements of 173.242 of this subchapter are applicable.
B52 - Notwithstanding the provisions of 173.24b of this subchapter, non-reclosing pressure relief devices are authorized on DOT 57 portable tanks.
IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).
T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3)
TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = $97 / 1 + a (tr - tf)$ Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.
TP29 - A portable tank having a minimum test pressure of 1.5 bar (150.0 kPa) may be used provided the calculated test pressure is 1.5 bar or less based on the MAWP of the hazardous materials, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.
DOT Packaging Exceptions (49 CFR 173.xxx) : 150
DOT Packaging Non Bulk (49 CFR 173.xxx) : 203
DOT Packaging Bulk (49 CFR 173.xxx) : 242
Marine pollutant : No

14.3. Additional information

Other information : No supplementary information available.
Special transport precautions : IMDG/IATA: NOT DANGEROUS GOODS.

Overland transport

Packing group (ADR) : III
Class (ADR) : 3 - Flammable liquid
Hazard identification number (Kemler No.) : 30
Classification code (ADR) : F1
Danger labels (ADR) : 3 - Flammable liquids



Orange plates :

Tunnel restriction code : D/E
Limited quantities (ADR) : 5L
EAC : •3YE
Excepted quantities (ADR) : E1

Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
MFAG-No : 127;128

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Air transport

DOT Quantity Limitations Passenger aircraft/rail : 60 L
(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 220 L

Civil Aeronautics Law : Flammable liquids

14.4. Environmental hazards

Other information : No supplementary information available.

14.5. Special precautions for user

Special transport precautions : IMDG/IATA: NOT DANGEROUS GOODS.

14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

BENZOIC ACID CALIBRANT FOR QNMR 5mM BENZOIC ACID IN DMSO-D6

SARA Section 311/312 Hazard Classes	Fire hazard Delayed (chronic) health hazard
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15.2. International regulations

CANADA

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Listed on the Canadian DSL (Domestic Substances List) inventory.

15.2.1. National regulations

No additional information available

15.3. US State regulations

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State or local regulations	U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.
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SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of R-, H- and EUH-phrases::

Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Skin Irrit. 2	skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H302	Harmful if swallowed
H315	Causes skin irritation
H318	Causes serious eye damage
H335	May cause respiratory irritation
R22	Harmful if swallowed
R37	Irritating to respiratory system
R37/38	Irritating to respiratory system and skin

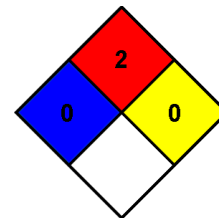
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R41	Risk of serious damage to eyes
Xi	Irritant
Xn	Harmful

- NFPA health hazard : 0 - Exposure under fire conditions would offer no hazard beyond that of ordinary combustible materials.
- NFPA fire hazard : 2 - Must be moderately heated or exposed to relatively high temperature before ignition can occur.
- NFPA reactivity : 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

- Health : 1 Slight Hazard - Irritation or minor reversible injury possible
- Flammability : 2 Moderate Hazard
- Physical : 0 Minimal Hazard

CIL Mixture SDS

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product