

# BENZOIC ACID CALIBRANT FOR QNMR 15mM BENZOIC ACID IN DMSO-D6 (750 UL FILL

# VOLUME)

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: 16/07/2015

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Version: 1.0

DLM-7061C

|   |  | ibstance/mixture and of the company/undertaking                                     |  |
|---|--|---|--|
| 1.1.                                    | Product identifier   |   |  |
| Produc                                  | t form   | : Mixtures  |  |
| Product name.                           |  | : BENZOIC ACID CALIBRANT FOR QNMR 15mM BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME) |  |
| Produc                                  | t code   | : DLM-7061C   |  |
| 1.2.                                    | Relevant identified uses of the sul  | bstance or mixture and uses advised against   |  |
| 1.2.1.                                  | Relevant identified uses   |   |  |
| Industr                                 | ial/Professional use spec  | : For professional use only.  |  |
| 1.2.2.                                  | Uses advised against   |   |  |
| No add                                  | litional information available   |   |  |
| 1.3.                                    | Details of the supplier of the safet   | y data sheet  |  |
| Andove<br>USA<br>USA:                   | ntage Road<br>er, MA 01810<br>1-800-322-1174 Int: 1-978-749-8000<br><u>s@isotope.com</u> www.isotope.com |   |  |
|   | Emergency telephone number   |   |  |
| Emerg                                   | ency numbers:  |   |  |
|   | rec: 1-800-424-9300 (24 hours)<br>tional: 1-703-741-5970 (24 hours)                                      |   |  |
| SECT                                    | TION 2: Hazards identification   |   |  |
| 2.1.                                    | Classification of the substance or   | mixture   |  |
| Skin Irı                                | fication according to Regulation (EC)<br>it. 2 H315<br>am. 1 H318  | No. 1272/2008 [CLP]   |  |
| STOT                                    | SE 3 H335  |   |  |
| Full tex                                | tt of H-phrases: see section 16  |   |  |
| Classi<br>Xi; R41<br>Xi; R37<br>Xi; R37 | 7  | /EEC or 1999/45/EC  |  |

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



2.3. **Other hazards** 

No additional information available

### **SECTION 3: Composition/information on ingredients**

Substances 3.1.

Not applicable

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| 3.2. Mixtures                            |   |                     |   |
|--|---|---------------------|---|
| Name                                     | Product identifier  | %                   | Classification according to<br>Directive 67/548/EEC                   |
| DIMETHYL SULFOXIDE-D6 (D, 99.9%)         | (CAS No) 2206-27-1<br>(EC no) 200-664-3                                     | 99.8463             | Not classified  |
| BENZOIC ACID UNLABELED                   | (CAS No) 65-85-0<br>(EC no) 200-618-2                                       | 0.1537              | Xn; R22<br>Xi; R41<br>Xi; R37   |
|  |   |                     |   |
| Name                                     | Product identifier  | %                   | Classification according to<br>Regulation (EC) No.<br>1272/2008 [CLP] |
| Name<br>DIMETHYL SULFOXIDE-D6 (D, 99.9%) | Product identifier           (CAS No) 2206-27-1           (EC no) 200-664-3 | <b>%</b><br>99.8463 | Regulation (EC) No.   |

#### 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   | <ul> <li>Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to<br/>do. Continue rinsing. Immediately call a POISON CENTER or doctor/physician.</li> </ul> |  |
| 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 eff   | ects, 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 media   | cal attention and special treatment needed   |  |
| No additional information available  |  |  |
| <b>SECTION 5: Firefighting measures</b>  |  |  |
| 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 s  | 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 me   |  |  |
| 6.1. Personal precautions, protective e  | 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 contain<br>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, includi   | ng 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/pers   | onal 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  | nronerties  |  |  |  |
|   |   |  |  |  |
|   | 9.1. Information on basic physical and chemical properties  |  |  |  |
| The properties listed below are for the solvent, the main compor  | nent of this mixture.   |  |  |  |
| The properties listed below are for the solvent, the main compor<br>Physical state  | ent of this mixture.<br>: Liquid  |  |  |  |
|   |   |  |  |  |
| Physical state  | : Liquid  |  |  |  |
| Physical state<br>Appearance  | : Liquid<br>: Liquid, clear.  |  |  |  |
| Physical state<br>Appearance<br>Color   | : Liquid<br>: Liquid, clear.<br>: Colourless.   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>301 °C (574 °F)</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>O data available</li> <li>No data available</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density<br>Solubility   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> <li>Water: Completely miscible</li> </ul>  |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density<br>Solubility<br>Log Pow  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density<br>Solubility<br>Log Pow<br>Log Kow   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density<br>Solubility<br>Log Pow<br>Log Kow<br>Viscosity, kinematic  | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>   |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density<br>Solubility<br>Log Pow<br>Log Kow<br>Viscosity, kinematic   | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul>      |  |  |  |
| Physical state<br>Appearance<br>Color<br>Odor<br>Odor threshold<br>pH<br>Relative evaporation rate (butyl acetate=1)<br>Melting point<br>Freezing point<br>Boiling point<br>Flash point<br>Self ignition temperature<br>Decomposition temperature<br>Flammability (solid, gas)<br>Vapor pressure<br>Relative vapor density at 20 °C<br>Relative density<br>Solubility<br>Log Pow<br>Log Kow<br>Viscosity, kinematic<br>Viscosity, dynamic<br>Explosive properties | <ul> <li>Liquid</li> <li>Liquid, clear.</li> <li>Colourless.</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>No data available</li> <li>18.4 °C (65.1 °F)</li> <li>No data available</li> <li>189 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> <li>301 °C (372 °F) at 1,013 hPa (760 mmHg)</li> <li>87 °C (189 °F) - closed cup</li> <li>301 °C (574 °F)</li> <li>No data available</li> </ul> |  |  |  |

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| 9.2. Other information  |  |  |  |
|---|--|--|--|
| No additional information available   |  |  |  |
| SECTION 10: Stability and reactivity  |  |  |  |
| 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 Hozardous decomposition products   |  |  |  |
| 10.6. Hazardous decomposition products<br>No additional information available |  |  |  |
|   |  |  |  |
| SECTION 11: Toxicological information   | on   |  |  |
| 11.1. Information on toxicological effects                                    |  |  |  |
| Acute toxicity  | : Not classified                               |  |  |
|   | M BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME) |  |  |
| 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%) (2206-2                                      | 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.                   |  |  |
| Symptoms/injuries after ingestion   | : May be harmful if swallowed.                 |  |  |
|   |  |  |  |

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| according to Regulation (EC) No. 453/2010 and according  | g to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations   |
|--|--|
| <b>SECTION 12: Ecological information</b>  |  |
| 12.1. Toxicity   |  |
| BENZOIC ACID CALIBRANT FOR QNMR 15m  | nM BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME)  |
| 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<br>ErC50 (algae)  | 17000 mg/l Pseudokirchneriella subcapitata (green algae) - 72 h<br>400000 mg/l Lepomis macrochirus (Bluegill) -96h   |
|  | 400000 mg/i Lepomis macrochirus (Biuegili) -901  |
| BENZOIC ACID UNLABELED (65-85-0)   |  |
| LC50 fish 1  | 180 mg/l Gambusia affinis (Mosquito fish) - 96 h   |
| 12.2. Persistence and degradability  |  |
|  | nM BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME)  |
| Persistence and degradability  | Not available.   |
| <b>,</b>   |  |
| DIMETHYL SULFOXIDE-D6 (D, 99.9%) (2206-<br>Persistence and degradability   | Not available.   |
| BOD (% of ThOD)  | 31 % ThOD  |
|  |  |
| BENZOIC ACID UNLABELED (65-85-0) Persistence and degradability   | Not available.   |
| • •  | NUT 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.   |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessme   |  |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessme   |  |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessment<br>No additional information available  | nt   |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessment<br>No additional information available<br>12.6. Other adverse effects   |  |
| Ecology - soil<br><b>12.5.</b> Results of PBT and vPvB assessment<br>No additional information available<br><b>12.6.</b> Other adverse effects<br>Other adverse effects  | nt<br>: Not available.   |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessment<br>No additional information available<br>12.6. Other adverse effects<br>Other adverse effects<br>SECTION 13: Disposal consideration  | nt<br>: Not available.   |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessment<br>No additional information available<br>12.6. Other adverse effects<br>Other adverse effects<br>SECTION 13: Disposal consideration<br>13.1. Waste treatment methods   | nt<br>: Not available.   |
| Ecology - soil<br>12.5. Results of PBT and vPvB assessment<br>No additional information available<br>12.6. Other adverse effects<br>Other adverse effects<br>SECTION 13: Disposal consideration<br>13.1. Waste treatment methods   | nt<br>: Not available.   |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)  | nt<br>: Not available.<br>IS<br>: Waste materials should be disposed of under conditions which meet Federal, State, and Local  |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations   | nt<br>: Not available.<br>S<br>: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.  |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information   | <ul> <li>nt</li> <li>Not available.</li> <li>Not available.</li> <li>S</li> <li>Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.</li> <li>Dispose in a safe manner in accordance with local/national regulations.</li> </ul>               |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information         In accordance with ADR / RID / ADNR / IMDG / IMD | <ul> <li>nt</li> <li>Not available.</li> <li>Not available.</li> <li>S</li> <li>Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.</li> <li>Dispose in a safe manner in accordance with local/national regulations.</li> </ul>               |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information         In accordance with ADR / RID / ADNR / IMDG / I         14.1.       UN number  | <ul> <li>nt</li> <li>Not available.</li> <li>Not available.</li> <li>S</li> <li>Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.</li> <li>Dispose in a safe manner in accordance with local/national regulations.</li> </ul>               |
| Ecology - soil  12.5. Results of PBT and vPvB assessment No additional information available  12.6. Other adverse effects Other adverse effects  SECTION 13: Disposal consideration 13.1. Waste treatment methods Regional legislation (waste)  Waste disposal recommendations  SECTION 14: Transport information In accordance with ADR / RID / ADNR / IMDG / I  14.1. UN number DOT NA no.   | nt<br>: Not available.<br>S<br>: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.<br>: Dispose in a safe manner in accordance with local/national regulations.<br>CAO / IATA   |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information         In accordance with ADR / RID / ADNR / IMDG / I         14.1.       UN number         DOT NA no.         14.2.       UN proper shipping name   | nt<br>: Not available.<br>S<br>: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.<br>: Dispose in a safe manner in accordance with local/national regulations.<br>CAO / IATA<br>NA1993   |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information         In accordance with ADR / RID / ADNR / IMDG / I         14.1.       UN number         DOT NA no.         14.2.       UN proper shipping name   | nt<br>: Not available.<br>S<br>: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.<br>: Dispose in a safe manner in accordance with local/national regulations.<br>CAO / IATA<br>NA1993<br>: Combustible liquid, n.o.s.                     |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information         In accordance with ADR / RID / ADNR / IMDG / I         14.1.       UN number         DOT NA no.         14.2.       UN proper shipping name         DOT Proper Shipping Name  | nt  : Not available.  S  : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.  : Dispose in a safe manner in accordance with local/national regulations.  CAO / IATA NA1993  : Combustible liquid, n.o.s. (Benzoic Acid, Dimethyl sulfoxide) |
| Ecology - soil         12.5.       Results of PBT and vPvB assessment         No additional information available         12.6.       Other adverse effects         Other adverse effects         SECTION 13: Disposal consideration         13.1.       Waste treatment methods         Regional legislation (waste)         Waste disposal recommendations         SECTION 14: Transport information         In accordance with ADR / RID / ADNR / IMDG / I         14.1.       UN number         DOT NA no.         14.2.       UN proper shipping name   | nt<br>: Not available.<br>S<br>: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.<br>: Dispose in a safe manner in accordance with local/national regulations.<br>CAO / IATA<br>NA1993<br>: Combustible liquid, n.o.s.                     |

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| DOT Symbols  | : D - Proper shipping name for domestic use only, or to and from Canada,G - Identifies PSN requiring a technical name   |
|--|---|
| Packing group (DOT)  | : III - Minor Danger  |
| DOT Special Provisions (49 CFR 172.102)                          | <ul> <li>IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HD2, 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).</li> <li>T1 - 1.5 178.274(d)(2) Normal</li></ul> |
| DOT Packaging Exceptions (49 CFR 173.xxx)                        | : 150   |
| DOT Packaging Non Bulk (49 CFR 173.xxx)                          | : 203   |
| DOT Packaging Bulk (49 CFR 173.xxx)                              | : 241   |
|  |   |
| 14.3. Additional information                                     |   |
| Other information  | : No supplementary information available.   |
| Special transport precautions                                    | : IMDG/IATA: NOT DANGEROUS GOODS.   |
| Overland transport   |   |
| No additional information available                              |   |
| 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   |
| Air transport  |   |
| DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) | : 60 L  |
| DOT Quantity Limitations Cargo aircraft only (49<br>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 Anne                        | ex 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 15mM BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME) |  |  |
| SARA Section 311/312 Hazard Classes   | Fire hazard<br>Delayed (chronic) health hazard |  |

### 15.2. International regulations

### CANADA

## BENZOIC ACID CALIBRANT FOR QNMR 15mM BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME)

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

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### 15.2.1. National regulations

No additional information available

### 15.3. US State regulations

| BENZOIC ACID CALIBRANT FOR QNMR 15mM BENZOIC ACID IN DMSO-D6 (750 UL FILL VOLUME)() |   |  |
|---|---|--|
| 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.  |  |

### **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                            |
| R41                 | Risk of serious damage to eyes                              |
| Xi                  | Irritant  |
| Xn                  | Harmful   |

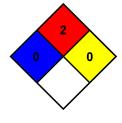
#### NFPA health hazard

NFPA fire hazard

NFPA reactivity

: 0 - Exposure under fire conditions would offer no hazard beyond that of ordinary combustible materials.

- : 2 Must be moderately heated or exposed to relatively high temperature before ignition can occur.
- : 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