


DR. J. PHARMACHEM (INDIA)

## MATERIAL SAFETY DATA SHEET

|     |  |   |
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| 1   | <b>IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING</b>        |   |
| 1.1 | <b>Product identifiers</b>   |   |
|     | Product Name   | Ambuphylline  |
|     | CAS NO.  | 5634-34-4   |
| 1.2 | <b>Relevant identified uses of the substance or mixture and uses advised against</b> |   |
|     | Identified uses  | Laboratory chemicals, Manufacture of substances                                     |
| 1.3 | <b>Details of the supplier of the safety data sheet</b>                              |   |
|     | COMPANY  | DR. J. PHARMACHEM (INDIA)   |
|     |  | 722/AB/15 'NIRMAL' ,LAXMI PARK COLONY,  |
|     |  | NAVI PETH , PUNE- 411 030.INDIA   |
|     |  | Telephone : 020-24530071  |
|     |  | Fax : 020-24530110  |
| 2   | <b>HAZARDS IDENTIFICATION</b>  |   |
| 2.1 | <b>Classification of the substance or mixture</b>                                    |   |
|     | <b>Classification according to Regulation (EC) No 1272/2008 [EU-GHS/CLP]</b>         |   |
|     | Acute toxicity, Oral (Category 3)  |   |
|     | <b>Classification according to EU Directives 67/548/EEC or 1999/45/EC</b>            |   |
|     | Harmful if swallowed.  |   |
| 2.2 | <b>Label elements</b>  |   |
|     | <b>Labelling according Regulation (EC) No 1272/2008 [CLP]</b>                        |   |
|     | Pictogram  |  |
|     | Signal word  | Danger  |
|     | Hazard statement(s)  |   |
|     | H301   | Toxic if swallowed.   |
|     | Precautionary statement(s)   |   |
|     | P301 + P310  | IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.                |



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|     | Supplemental Hazard Statements  | none  |
|     | <b>According to European Directive 67/548/EEC as amended</b>                      |   |
|     | Hazard symbol(s)  | <b>X</b>  |
|     | R-phrase(s)   |   |
|     | R22   | Harmful if swallowed.   |
|     | S-phrase(s)   | none  |
| 2.3 | <b>Other hazards</b>  | none  |
| 3   | <b>COMPOSITION/INFORMATION ON INGREDIENTS</b>                                     |   |
| 3.1 | <b>Substances</b>   |   |
|     | Synonyms  | Theophylline-2-aminoisobutanol  |
|     | Formula   | C <sub>11</sub> H <sub>19</sub> N <sub>5</sub> O <sub>3</sub>   |
|     | Molecular Weight  | 269.3003  |
|     | Component   | Concentration   |
|     | Ambuphylline  | Min 98%   |
|     | Other unknown impurities  | Up to 2%  |
| 4   | <b>FIRST AID MEASURES</b>   |   |
| 4.1 | <b>Description of first aid measures</b>  |   |
|     | <b>General advice</b>   | Consult a physician. Show this safety data sheet to the doctor in attendance.                                   |
|     | <b>If inhaled</b>   | If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician. |
|     | <b>In case of skin contact</b>  | Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.               |
|     | <b>In case of eye contact</b>   | Flush eyes with water as a precaution.  |
|     | <b>If swallowed</b>   | Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.             |
| 4.2 | <b>Most important symptoms and effects, both acute and delayed</b>                |   |
|     | Nausea, Vomiting, Headache, Diarrhoea, Epigastric pain., Circulatory collapse     |   |
| 4.3 | <b>Indication of any immediate medical attention and special treatment needed</b> |   |
|     | No data available   |   |
| 5   | <b>FIREFIGHTING MEASURES</b>  |   |
| 5.1 | <b>Extinguishing media</b>  |   |
|     | <b>Suitable extinguishing media</b>   | Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.  |
| 5.2 | <b>Special hazards arising from the substance or mixture</b>                      | Carbon oxides, nitrogen oxides (NO <sub>x</sub> )   |
| 5.3 | <b>Advice for firefighters</b>  | Wear self contained breathing apparatus for firefighting if necessary.  |
| 5.4 | <b>Further information</b>  | No data available   |
| 6   | <b>ACCIDENTAL RELEASE MEASURES</b>  |   |
| 6.1 | <b>Personal precautions, protective equipment and emergency procedures</b>        |   |



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|     | Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.  |
| 6.2 | <b>Environmental precautions</b>  |
|     | Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.  |
| 6.3 | <b>Methods and materials for containment and cleaning up</b>  |
|     | Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.  |
| 6.4 | <b>Reference to other sections</b>  |
|     | For disposal see section 13.  |
| 7   | <b>HANDLING AND STORAGE</b>   |
| 7.1 | <b>Precautions for safe handling</b>  |
|     | Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.   |
| 7.2 | <b>Conditions for safe storage, including any incompatibilities</b>   |
|     | Store in cool place. Keep container tightly closed in a dry and well-ventilated place.  |
| 7.3 | <b>Specific end uses</b>  |
|     | no data available   |
| 8   | <b>EXPOSURE CONTROLS/PERSONAL PROTECTION</b>  |
| 8.1 | <b>Control parameters</b>   |
|     | <b>Components with workplace control parameters</b>   |
| 8.2 | <b>Exposure controls</b>  |
|     | <b>Appropriate engineering controls</b>   |
|     | Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.  |
|     | <b>Personal protective equipment</b>  |
|     | <b>Eye/face protection</b>  |
|     | Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  |
|     | <b>Skin protection</b>  |
|     | Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.<br>The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it. |
|     | <b>Body Protection</b>  |
|     | Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace  |
|     | <b>Respiratory protection</b>   |
|     | Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).                            |
| 9   | <b>PHYSICAL AND CHEMICAL PROPERTIES</b>   |
| 9.1 | <b>Information on basic physical and chemical properties</b>  |



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|      |   |  |
|------|---|--|
| a)   | Appearance                                  | Form : Crystalline powder<br>Colour :White   |
| b)   | Odour                                       | Like Amine   |
| c)   | Odour Threshold                             | No data available  |
| d)   | pH  | No data available  |
| e)   | Melting range/freezing range                | No data available  |
| f)   | Initial boiling point and boiling range     | 454.1 °C at 760 mmHg   |
| g)   | Flash point                                 | 228.4 °C   |
| h)   | Enthalpy of Vaporization                    | 71.36 kJ/mol   |
| i)   | Index of Refraction                         | No data available  |
| j)   | Molar Refractivity                          | No data available  |
| k)   | Vapour pressure                             | 1.96E-08 mmHg at 25 °C   |
| l)   | Density                                     | No data available  |
| m)   | Oxidizing properties                        | No data available  |
| n)   | Water solubility                            | Freely soluble   |
| o)   | Partition coefficient: noctanol/water       | No data available  |
| p)   | Polarizability                              | No data available  |
| q)   | Decomposition temperature                   | No data available  |
| r)   | Molar Volume                                | No data available  |
| s)   | Surface Tension                             | No data available  |
| 9.2  | <b>Other safety information</b>             |  |
|      | IUPAC Name                                  | 2-amino-2-methylpropan-1-ol  |
|      | Molecular Formula                           | C <sub>11</sub> H <sub>19</sub> N <sub>5</sub> O <sub>3</sub>  |
|      | Molecular Weight                            | 269.3003   |
|      | SMILES                                      | O=C2N(c1ncnc1C(=O)N2C)C.OCC(N)(C)C   |
|      | InChI                                       | InChI=1/C7H8N4O2.C4H11NO/c1-10-5-4(8-3-9-5)6(12)11(2)7(10)13;1-4(2,5)3-6/h3H,1-2H3(H,8,9);6H,3,5H2,1-2H3   |
|      | EINECS                                      | 227-077-5  |
| 10   | <b>STABILITY AND REACTIVITY</b>             |  |
| 10.1 | <b>Reactivity</b>                           | no data available  |
| 10.2 | <b>Chemical stability</b>                   | no data available  |
| 10.3 | <b>Possibility of hazardous reactions</b>   | no data available  |
| 10.4 | <b>Conditions to avoid</b>                  | no data available  |
| 10.5 | <b>Incompatible materials</b>               | Strong oxidizing agents  |
| 10.6 | <b>Hazardous decomposition products</b>     | Other decomposition products - no data available   |
| 11   | <b>TOXICOLOGICAL INFORMATION</b>            |  |
| 11.1 | <b>Information on toxicological effects</b> |  |
|      | <b>Acute toxicity</b>                       | LD50 Oral - rat - 225 mg/kg<br>LC50 Inhalation - rat - male and female - 4 h - > 6,7 mg/l<br>LD50 Dermal - rat - male and female - > 2.000 mg/kg |
|      | <b>Skin corrosion/irritation</b>            | Skin - rabbit - No skin irritation - OECD Test Guideline 404   |



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|      | <b>Serious eye damage/eye irritation</b>   | Eyes - rabbit - No eye irritation - OECD Test Guideline 405   |
|      | <b>Respiratory or skin sensitization</b>   | no data available   |
|      | <b>Germ cell mutagenicity</b>  | Laboratory experiments have shown mutagenic effects.  |
|      | <b>Carcinogenicity</b>   | This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.<br>IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans |
|      | <b>Reproductive toxicity</b>   | Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.   |
|      | <b>Specific target organ toxicity - single exposure</b>  | no data available   |
|      | <b>Specific target organ toxicity - repeated exposure</b>  | no data available   |
|      | <b>Aspiration hazard</b>   | no data available   |
|      | <b>Potential health effects</b>  |   |
|      | <b>Inhalation</b>  | May be harmful if inhaled. May cause respiratory tract irritation.  |
|      | <b>Ingestion</b>   | Toxic if swallowed.   |
|      | <b>Skin</b>  | May be harmful if absorbed through skin. May cause skin irritation.   |
|      | <b>Eyes</b>  | May cause eye irritation.   |
|      | <b>Signs and Symptoms of Exposure</b>  |   |
|      | Nausea, Vomiting, Headache, Diarrhoea, Epigastric pain., Circulatory collapse  |   |
|      | <b>Additional Information</b>  |   |
|      | RTECS  | XH3850000   |
| 12   | <b>ECOLOGICAL INFORMATION</b>  |   |
| 12.1 | <b>Toxicity</b>  | no data available   |
|      | Toxicity to fish   | LC50 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h   |
|      | Toxicity to daphnia and other aquatic invertebrates  | EC50 - Daphnia magna (Water flea) - 178 mg/l - 48 h   |
|      | Toxicity to algae  | EC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l -72 h   |
| 12.2 | <b>Persistence and degradability</b>   | Biodegradability Biotic/Aerobic<br>Result: > 90 - 100 % - Readily biodegradable.  |
| 12.3 | <b>Bioaccumulative potential</b>   | no data available   |
| 12.4 | <b>Mobility in soil</b>  | no data available   |
| 12.5 | <b>Results of PBT and vPvB assessment</b>  | no data available   |
| 12.6 | <b>Other adverse effects</b>   | no data available   |
| 13   | <b>DISPOSAL CONSIDERATIONS</b>   |   |
| 13.1 | <b>Waste treatment methods</b>   |   |
|      | <b>Product</b>   |   |
|      | Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. |   |



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|      | <b>Contaminated packaging</b>   |                                 |                              |
|      | Dispose of as unused product.   |                                 |                              |
| 14   | <b>TRANSPORT INFORMATION</b>  |                                 |                              |
| 14.1 | <b>UN number</b>  |                                 |                              |
|      | ADR/RID   | IMDG                            | IATA                         |
|      | 2811  | 2811                            | 2811                         |
| 14.2 | <b>UN proper shipping name</b>  |                                 |                              |
|      | ADR/RID   | IMDG                            | IATA                         |
|      | TOXIC SOLID, ORGANIC,<br>N.O.S.   | TOXIC SOLID, ORGANIC,<br>N.O.S. | Toxic solid, organic, n.o.s. |
| 14.3 | <b>Transport hazard class(es)</b>   |                                 |                              |
|      | ADR/RID   | IMDG                            | IATA                         |
|      | 6.1   | 6.1                             | 6.1                          |
| 14.4 | <b>Packaging group</b>  |                                 |                              |
|      | ADR/RID   | IMDG                            | IATA                         |
|      | III   | III                             | III                          |
| 14.5 | <b>Environmental hazards</b>  |                                 |                              |
|      | ADR/RID   | IMDG Marine pollutant           | IATA                         |
|      | no  | no                              | no                           |
| 14.6 | <b>Special precautions for user</b>   |                                 |                              |
|      | no data available   |                                 |                              |
| 15   | <b>REGULATORY INFORMATION</b>   |                                 |                              |
|      | This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.  |                                 |                              |
| 15.1 | <b>Safety, health and environmental regulations/legislation specific for the substance or mixture</b>   |                                 |                              |
|      | no data available   |                                 |                              |
| 15.2 | <b>Chemical Safety Assessment</b>   |                                 |                              |
|      | no data available   |                                 |                              |
| 16   | <b>OTHER INFORMATION</b>  |                                 |                              |
|      | <b>Further information</b>  |                                 |                              |
|      | <p>The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Dr J Pharmachem (India) and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See <a href="http://www.jpharmachem.com">www.jpharmachem.com</a> and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.</p> <p>Month of creation :- October 2013<br/>Month of revision :- October 2016</p> |                                 |                              |