

1,2,6-Hexanetriol (1,2,6-trihydroxyhexane)

PRODUCT No.
T6,620-6

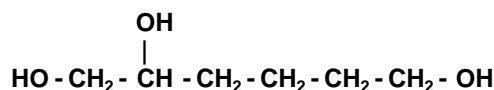
revised 4 / 96

2 pages

INTRODUCTION

The Aldrich Group of Companies is one of the world's major multinational producers and suppliers of fine organic chemicals and intermediates.

Worldwide, the Group produces over 2,000 organic compounds, many on a tonnage scale. These high-quality chemicals are used for research, analysis, synthesis, industrial production and as pharmaceutical intermediates. As demand for a chemical increases, every effort is made to ensure a continuous supply. 1,2,6-Hexanetriol is an example.



Aldrich has been a source of 1,2,6-hexanetriol in ton quantities for many years but the increasing demand for this versatile chemical finally outgrew our supply capabilities. However, production has now been scheduled to enable us to ensure on-going supplies of very high quality (98+%) material in multiton quantities.

1,2,6-Hexanetriol has an interesting combination of attractive properties:

- Liquid polyol
- Miscible with water
- High boiling point
- Stable
- Non-toxic

1,2,6-Hexanetriol has been used mainly in cosmetic and pharmaceutical preparations and in a wide variety of applications in the plastics industry. The availability of 1,2,6-hexanetriol in large quantities will lead inevitably to the development of many new applications.

PROPERTIES

Molecular formula	C ₆ H ₁₄ O ₃
Molecular weight	134.17
Purity (hydroxyl titration)	98+%
Color	colorless to faintly yellow
Boiling point	178°C / 5mm Hg
Flash point	79°C (175°F)
Specific gravity	1.109
Refractive index, n_D^{20}	1.478
Surface tension at 20°C	50 dynes / cm
Solubility at 20°C:		
Water	miscible (A 30% by weight aqueous solution is clear without any cloudiness or non-miscible matter.)	
actone	miscible	
octane	< 0.2% by weight	
toluene	< 0.2% by weight	
Viscosity at		
20°C	2630 centipoises	
30°C	1095 centipoises	

The general properties of 1,2,6-hexanetriol, which has primary and secondary alcohol groups, are similar to those of other polyols in which the hydroxyl groups are situated on different carbon atoms. Such compounds are relatively stable and because of the considerable intermolecular association due to the multiplicity of polar hydroxyl groups and hydrogen bonding, they have high boiling points, are hygroscopic in nature, and have considerable water solubility but low solubility in non-polar solvents.

1,2,6-Hexanetriol resembles, in many ways, glycerol, the most well known triol which is the major constituent of animal fats. By comparison, hexanetriol is more viscous, has a lower density, and is about half as hygroscopic as glycerol. There are, of course, many other subtle differences in physical and chemical behavior associated with the larger molecule of 1,2,6-hexanetriol.

APPLICATIONS

The interesting physical and chemical properties of 1,2,6-hexanetriol have led to a wide variety of applications. It finds use as a versatile solvent or constituent of mixtures and in a variety of chemical coupling reactions of particular importance in the resin / plastics industry.

SOLVENT / MIXTURES

1,2,6-Hexanetriol is making in-roads to fields where glycerol is well established. For many applications, the improved performance properties of 1,2,6-hexanetriol more than justify its higher cost. Thus, 1,2,6-hexanetriol, because of its "more organic" (higher C : OH ratio) and bulkier molecule as compared with glycerol, we, in certain cases, result in more compatible mixtures / emulsions, especially with non-polar compounds. For the same reason, it exhibits good plasticizing properties.

Pharmaceutical / Cosmetic - 1,2,6-Hexanetriol is now used as a humectant (moisturizing agent) for various creams and toiletries. It is, in fact, the preferred solvent base for many steroids in cream applications.

Inks / Paints - The excellent solvent properties of 1,2,6-hexanetriol have resulted in its use as the carrier solvent for ball-point pen inks, in printing inks and a variety of paint formulations. Compared with glycerol, 1,2,6-hexanetriol is more viscous and gives better pigment dispersion.

Possible Applications - 1,2,6-Hexanetriol will probably find application as a solvent in the photography and textile industries.

1,2,6-Hexanetriol has considerable potential as a solvent in aerosols.

There are also possibilities in various diverse outlets, e.g., as a humectant in tobacco, as a plasticizer for cellophane, and in glue formulations.

RESINS / PLASTICS

1,2,6-Hexanetriol has been used in the manufacture of various synthetic resins. These applications utilize the ability of 1,2,6-hexanetriol to cross-link with other chemicals via its -OH groups. It is envisaged that major outlets will develop for specialized applications where one needs to incorporate a bulky molecule into the system to achieve the required end-use properties.

Alkyd Resins - 1,2,6-Hexanetriol gives resins which have lower viscosities than those of glycerol, thus allowing a higher solid content in certain ink and enamel formulations.

Plasticizers - Various esters of 1,2,6-hexanetriol have proven to be excellent plasticizers which have found application not only for plastics, e.g., PVC and cellulose acetate, but also for certain rubbers, e.g., nitrile and neoprene.

Polyurethanes - 1,2,6-Hexanetriol has been employed in a variety of polyurethane systems. Thus, it can be simply used as the cross-linking polyol with isocyanates. In combination with propylene oxide, it has been used to produce both flexible and rigid urethane foams.

HANDLING

PACKAGING

1,2,6-Hexanetriol is supplied in drums which allow safe storage and do not discolor the chemical.

HAZARD



(F) FLAMMABLE



(XN) HARMFUL

Inasmuch as our affiliated European companies have sold many tons of this product, we have classified the chemical according to the West European coding F + Xn. The F (Flammable) designation is obvious - the material burns - whereas Xn (Harmful) may appear inconsistent with its known non-toxic properties. However, glycerol, which closely resembles 1,2,6-hexanetriol in its toxic behavior has been classified Xn by the West European authorities, indicating the emphasis on bringing to the attention of the end user, even the slightest possible health hazard. We fully support this cautious approach and thus have similarly designated the compound as Xn.

TOXICITY

Investigation suggests 1,2,6-hexanetriol can be classified as virtually non-toxic. Its oral toxicity for rats (LD50 16g/kg, NIOSH Registry of Toxic Effects of Chemical Substances) is less than that of ethyl alcohol and only slightly higher than for glycerol. Rats fed up to 10% hexanetriol in their diet showed no adverse effects. It also caused no reaction when applied to the skin of rabbits.

The customary care in handling chemicals should be taken. Thus, all handlers should wear protective clothing, i.e., safety glasses and gloves, and work should be carried out in areas of adequate ventilation.

EMERGENCY

Spills - The liquid should be absorbed either by vermiculite or other absorbent material and placed in a closed container. The material should then be disposed of by burning. Any trace of liquid remaining should be washed down with water and soap or detergent.

Eyes affected - Wash thoroughly and continuously with water until medical attention is obtained.

Skin contact - Wash well with running water and soap or detergent.

FIRE

Extinguish with water, dry powder or carbon dioxide.

1,2,6-Hexanetriol is a very interesting chemical which has found use in a wide variety of applications. If you have any questions, please contact us at your convenience. We shall be pleased to place our expertise at your service.

Material will be billed at the price in effect at the time shipment is made.

Inquiries for bulk quantities of 1,2,6-hexanetriol for drug testing or manufacturing purposes in accordance with the Federal Food, Drug and Cosmetic Act are invited and will be considered on an individual basis.

Aldrich Chemical Company, Inc.

1001 West Saint Paul Ave., Milwaukee, WI 53233

Telephone 414-273-3850

Fax 414-273-4979

Internet aldrich@sial.com

800-231-8327

800-962-9591

Aldrich warrants that its products conform to the information contained in this and other Aldrich publications. Purchaser must determine the suitability of the product for its particular use. See reverse side of invoice or packing slip for additional terms and conditions of sale.

