Shell Chemicals

**Data Sheet**

**Issued:**

16-Mar-2007

**Product Name**

# Butyl OXITOL

**Product Code**

**U5117**

**Product Category**

**Ethylene Glycol Ethers**

**CAS Registry Number** 111-76-2

**EINECS Number** 203-905-0

**Alternate Name** 2-butoxyethanol, BuOX, BG

**Description**

Butyl OXITOL is a colourless, mild smelling liquid with a high boiling point. It is slightly hygroscopic and miscible with water at room temperature. At higher temperatures a miscibility gap with water occurs in the system. Butyl OXITOL is also miscible with numerous oxygenated solvents, as well as with aliphatic and aromatic hydrocarbons and oils; it has outstanding solvent power for many nature and synthetic resins, nitrocellulose and ethyl cellulose. Butyl OXITOL forms binary azeotropic mixtures with water and a range of organic substances.

**Sales Specification**

| Property | Unit | Min | Max | Method | |
|---|---|---|---|---|---|
| Purity | %m/m | 99.0 | | DIN 55688 | |
| Water | %m/m | | 0.10 | ASTM D1364 | |
| Acidity as Acetic acid | %m/m | | 0.005 | ASTM D1613 | |
| Peroxides as O | mg/kg | | 10 | SMS 359 | |
| Appearance | Clear & Free From Suspended Matter | | | ASTM D4176 | |
| Color | Pt-Co | | 10 | ASTM D1209 | |
| Density @20°C | g/mL | 0.898 | 0.902 | ASTM D4052 | (4) |
| Refractive Index @20°C | | | | ASTM D1218 | (2) |
| Distillation, IBP | °C | | | ASTM D1078 | (2) |
| Distillation, DP | °C | | | ASTM D1078 | (2) |

(2) Typical / Representative value provided

(4) Agreed Specification limits - no results: Statistical average value reported

## Typical Properties

| Property | Unit | Method | Value |
|---|---|---|---|
| Purity | % m/m | DIN 55688 | min. 99.0 |
| Water | % m/m | ASTM D1364 | 0.05 |
| Density @20°C | kg/L | ASTM D4052 | 0.900 |
| Cubic Expansion Coefficient @20°C | (10^-4)/°C | Calculated | 9 |
| Refractive Index @20°C | - | ASTM D1218 | 1.419 |
| Color | Pt-Co | ASTM D1209 | < 5 |
| Boiling Point | °C | - | 171 |
| Relative Evaporation Rate (nBuAc=1) | - | ASTM D3539 | 0.08 |
| Relative Evaporation Rate (Ether=1) | - | DIN 53170 | 160 |
| Antoine Constant A # | kPa, °C | - | 6.95668 |
| Antoine Constant B # | kPa, °C | - | 1920.77 |
| Antoine Constant C # | kPa, °C | - | 217.774 |
| Antoine Constants: Temperature range | °C | - | +30 to +170 |
| Vapor Pressure @20°C | kPa | Calculated | 0.08 |
| Vapor Pressure @50°C | kPa | Calculated | 0.61 |
| Saturated Vapor Concentration @20°C | g/m³ | Calculated | 4 |
| Flash Point | °C | ASTM D93 | 67 |
| Auto Ignition Temperature | °C | ASTM E659 | 240 |
| Explosion Limit: Lower | %v/v | - | 1.1 |
| Explosion Limit: Upper | %v/v | - | 10.6 |
| Electrical Conductivity @20°C | µS/m | ASTM D4308 | 10 |
| Dielectric Constant @20°C | - | - | 9.4 |
| Freezing Point | °C | - | -70 |
| Surface Tension @20°C | mN/m | - | 28 |
| Viscosity @20°C | mPa.s | ASTM D445 | 3.3 |
| Hildebrand Solubility Parameter | (cal/cm³)^½ | - | 9.1 |
| Hydrogen Bonding Index | - | - | 0.0 |
| Fractional Polarity | - | - | 0.048 |
| Dilution Ratio: Toluene | - | ASTM D1720 | 3.3 |
| Dilution Ratio: SBP 100/140 | - | ASTM D1720 | 1.9 |
| Heat of Vaporization @Tboil | kJ/kg | - | 365 |
| Heat of Combustion (Net) @25°C | kJ/kg | - | 30500 |
| Specific Heat @20°C | kJ/kg/°C | - | 2.4 |
| Thermal Conductivity @20°C | W/m/°C | - | 0.17 |
| Miscibility @20°C: Solvent in Water | % m/m | - | Complete |
| Miscibility @20°C: Water in Solvent | % m/m | - | Complete |
| Azeotrope with Water: Boiling Point | °C | - | 98.8 |
| Azeotrope with Water: Solvent Content | % m/m | - | 20.8 |
| Molecular Weight | g/mol | - | 118 |

(#) In the Antoine temperature range, the vapor pressure P (kPa) at temperature T (°C) can be calculated by means of the Antoine equation: log P = A - B/(T+C)

| | |
|---|---|
| **Test Methods** | Copies of copyrighted test methods can be obtained from the issuing organisations:<br><br>American Society for Testing and Materials (ASTM) : www.astm.org<br>Energy Institute (IP) : www.energyinst.org.uk<br>Deutsches Institut für Normung (DIN) : www.din.de<br><br>For routine quality control analyses, local test methods may be applied that are different from those mentioned in this datasheet. Such methods have been validated and can be obtained through your local Shell Chemicals company. |
| **Quality** | Butyl OXITOL can be supplied to meet the requirements of ASTM D330, DIN 55999 and BS 509. |
| **Storage and Handling** | Provided proper storage and handling precautions are taken we would expect Butyl OXITOL to be technically stable for at least 12 months. For detailed advice on Storage and Handling please refer to the Material Safety Data Sheet on www.shell.com/chemicals. |
| **Hazard Information** | For detailed Hazard Information please refer to the Material Safety Data Sheet on www.shell.com/chemicals. |
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