Technical Information

TBAc™ Solvent

(Tertiary Butyl Acetate)
CAS No. 540-88-5

Description

TBAc solvent is Lyondell Chemical Company's brand of tert-butyl acetate, a VOC (volatile organic compound)-exempt[1], non-HAP (hazardous air pollutant), urethane-grade solvent with low toxicity. It has a characteristic ester odor and is soluble in water to the extent of 0.8% at 23°C. It has excellent solvency for a variety of substances including nitrocellulose, acrylic, alkyd, polyester and urethane resins. TBAc solvent is a substitute for a variety of HAP and VOC solvents including toluene, xylene, esters, ketones and hydrocarbons.

Product Identification

Chemical Name .... acetic acid, 1,1-dimethylethyl ester
Chemical Family ..... aliphatic ester
Other Names ..... acetic acid, tert-butyl ester
..... 1,1-dimethylethyl acetate
..... tertiary-butyl alcohol, acetate
..... 2-acetoxy-2-methylpropane
Chemical Formula ..... $C_6H_{12}O_2$

*Product Specifications

Property	Specifications	Test Method
Acidity, wt. % as acetic acid, max.	0.01	ASTM D-1613
Water, wt. %, max.	0.05	ASTM E-203
Color, APHA, max.	10	ASTM E-1209
GC purity, wt. %, min.	99.5	Internal Method

* For the most current product specification, please call 1-888-777-0232 in North America; 33-3-44-24-9204 in Europe or check www.tbac.com.

Typical Properties

- Autoignition temperature (°C).....518
- Density (g/ml @ 25°C) (lbs./gal).....0.8599 (7.18)
- Evaporation rate (BuAc = 100).....280
- Flammability limits (lower/upper vol. %).....1.26/6.88
- Flash Point (Tag Closed Cup) °C (°F).....4.4 (40)
- Solubility by weight in water @ 23°C.....0.8%
- Maximum incremental reactivity (MIR).....0.20g ozone/gTBAc
- Dielectric constant (DIC @20°C, cyclohexane) 1.94
- Solubility parameter (total Hansen).....7.7
- Surface tension (dynes/cm) @ 20°C (68°F).....22.4
- Electrical resistivity (megaOhms).....23.8
- Viscosity (centistokes) @20°C (68°F).....<1.2
- Vapor pressure @ 20°C (mm Hg).....31
- Boiling point @ 760mm Hg.....98°C

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Applications

Coatings, Inks, Adhesives: TBAc solvent finds use in decorative and industrial coating formulations, packaging inks and pressure-sensitive adhesives. It is a useful tool in the formulation of VOC- and HAP-compliant coatings, inks and adhesives. TBAc solvent is less volatile and flammable than exempt acetone and methyl acetate.

TBAc solvent has a similar evaporation rate and solvency as MEK, MIBK, ethyl and propyl acetate, and toluene in a variety of coating systems, including 2K urethanes, alkyds, acrylics, nitrocellulose lacquers and baking enamels. Because of its superior resistance to amines, TBAc solvent can also be used in epoxy polyamide coatings as a replacement for toluene.

Cleaners: For solvent-based cleaning, including metal degreasing and specialized equipment cleansing, TBAc solvent improves the cleaning efficiency of toluene, mineral spirits and acetone on baked-on greasy soil and lithium grease. TBAc solvent is non-halogenated and cannot deplete the ozone layer. TBAc solvent shows very broad solvency. Its solvency characteristics generally match those of chlorinated solvents and hydrocarbons.

Electronics: Another area where TBAc solvent may replace other solvents is in photoresist formulations used in semiconductor processing. In these processes, it is used in positive photoresist formulations. TBAc solvent may also be used in solvent systems for cleaning and degreasing circuit boards and removing solder flux.

Other Applications: The properties listed in the previous section also support the use of TBAc solvent in agricultural and textile products. It is a useful intermediate in the pharmaceutical industry.

Storage

General industry practice is to store TBAc solvent in carbon steel vessels.

Store only in tightly closed, properly vented containers away from heat, sparks, open flame or strong oxidizing agents. Use only non-sparking tools. Ground containers before beginning transfer. Electrical equipment should conform to national electric code.

Safety and Handling

Handle empty containers carefully. Store in properly lined steel or stainless steel to avoid slight discoloration from mild steel. This product may absorb water if exposed to air.

TBAc solvent has a flash point of 40°F (4.4°C). It is a flammable liquid as defined under SARA Title III, section 311/312 hazard category but is not subject to the reporting requirements of SARA Title III, section 313.

Undue exposure or spillage should be strictly avoided as a matter of good practice. Refer to the Material Safety Data Sheet for more specific information.

Hazard ratings are summarized as follows:

	NPCA HMIS	NFPA
Health	1	1
Flammability	3	3
Reactivity	0	0

Personal protection recommendation should be made with consideration of specific work place conditions. The health hazard rating is based on eye irritation potential.

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Toxicological Evaluation

TBAc solvent has a low degree of acute toxicity. The oral LD50 is 4.5 g/kg and the inhalation LC50 for six hours of exposure is approximately 4200 ppm. It is a moderate skin and eye irritant. A battery of genotoxicity studies was negative. Inhalation of 1600 ppm TBAc solvent by rats for two weeks resulted in unsteady gait and liver toxicity; increased hyaline droplets were found in the kidneys of male rats exposed at 100, 400 and 1600 ppm.

Pharmacokinetic studies indicate a portion of TBAc solvent is metabolized to its parent alcohol, TBA. TBA has been demonstrated to cause alpha-2U-globulin toxicity in male rat kidneys. As a matter of safe practice, ingestion and prolonged skin contact should be avoided. Refer to the Material Safety Data Sheet for more specific information.

Regulatory Status

The U.S. EPA has added tertiary butyl acetate to the list of VOC-exempt [1] compounds based on its negligible photochemical reactivity and negligible contribution to tropospheric ozone.

TBAc solvent is not subject to the reporting requirement of CERCLA or the reporting requirements established by SARA Title III, section 313 and 40CFR372.

TBAc solvent is on the U.S. TSCA inventory, Canadian DSL (Jan 26, 1991), Australian AICS, Korean ECL (KE-04180), European EINECS (208-760-7) and ENCS (2-731X), Swiss Giftliste 1 (G-3350), PICCS and ASIA-PAC lists.

Refer to the Material Safety Data Sheet for more specific information.

Material Compatibility Guidelines

Stainless steel is recommended for valves, pumps and filters. Teflon®[2] is suitable for gaskets. Natural rubber, ABS, silicone, Viton and Neoprene are known to swell in contact with TBAc solvent. Information from material suppliers and specific conditions of contact should be considered in the selection of suitable materials.

[1] The U.S. EPA has published a rule excluding tertiary butyl acetate from the Federal definition of a VOC (40 C.F.R. § 51.100(s)(5); see also 69 FR 69304).

[2] Teflon is a registered trademark of E. I. duPont de Nemours and Company.

World Headquarters
Lyondell Chemical Company
1221 McKinney
Houston, TX 77010
Tel (713) 652-7200
Toll-free (888) 777-0232
MSDS Hotline: (800) 700-0946

European Headquarters
Lyondell Chemical Europe, Inc.
P. O. Box 2416
3000 CK Rotterdam
The Netherlands
Tel (31) 10 275-5500
Tel (33) 3 44 24 92 05 (tech svc)

Lyondell South America
Av Roque Petroni Jr,
999, cj 123
Sao Paulo, SP 04707-910
Brazil
Tel (55) 11-5185-9300

Asian Headquarters
Lyondell Asia Pacific, Ltd.
41st Floor – The Lee Gardens
33 Hysan Avenue
Causeway Bay, Hong Kong
Tel (852) 28822-668
Tel (33) 3 44 24 92 05 (tech svc)

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