

Technical Data

TBAc™ Solvent

(Tertiary Butyl Acetate) Environmental Aspects

Introduction

TBAc solvent, Lyondell Chemical Company's brand of tert-butyl acetate, CAS# 540-88-5, is a unique non-HAP (hazardous air pollutant), VOC (volatile organic compound)-exempt* organic solvent with versatile performance and negligible photochemical activity. It is suitable for use in coatings, inks, adhesives, and cleaners. It is a potential substitute for a variety of HAP solvents and VOCs such as toluene, xylene, MEK, and MIBK as well as ozone depleting solvents such as methyl chloroform and CFC-113.

Unless otherwise noted, the following environmental fate information was taken from the US National Library of Medicine's HSDB database¹ and the references contained therein.

Summary

Because of its high vapor pressure and low water solubility, tert-butyl acetate will degrade in the environment primarily by atmospheric oxidation.

If released to soil, tert-butyl acetate will rapidly leach out and volatilize. If released to water, the majority of tert-butyl acetate will volatilize within days and the rest will biodegrade within weeks. Aquatic adsorption and bio-concentration will, therefore, not be significant.

The atmospheric fate of tert-butyl acetate is well understood. In a typical atmosphere, it reacts with atmospheric OH radicals with a half-life of 26 days. In a polluted atmosphere, it oxidizes to acetic anhydride, acetone, and organic nitrates, which, in turn, ultimately oxidize to CO₂ and water.

Because of their high affinity for water, acetic anhydride and acetone will be efficiently removed via washout and, ultimately, biodegrade.

Tert-butyl acetate is negligibly photo-reactive, generating less than 70% the amount of ozone produced by ethane on a per gram basis. Tert-butyl acetate and its photoproducts also exist predominantly in the vapor phase in the atmosphere and are, therefore, not aerosol or particulate precursors.

Tert-butyl acetate does not contain halogens and cannot, therefore, deplete stratospheric ozone. Tert-butyl acetate also does not contain nitrogen or sulfur and will not contribute appreciably to acid rain in the form of nitric, halo, or sulfuric acids.

Atmospheric Fate

Aerosol Forming Potential - Tert-butyl acetate will exist almost entirely in the vapor-phase in the ambient atmosphere due to its high vapor pressure (34 mm Hg @25°C). Its photoproducts are also volatile and are not expected to generate aerosols of fine particulate matter (PM_{2.5}).²

Global Warming Potential - The half-life for the vapor-phase reaction of tert-butyl acetate with atmospheric hydroxyl radicals is about 26 days in an average atmosphere. Based on this short atmospheric lifetime, tert-butyl acetate is not expected to contribute significantly to global warming.³

Tert-butyl acetate is a member of the ester class of chemicals whose global warming potential was reviewed under SNAP and considered not to be of concern.⁴

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Ozone Forming Potential – Tert-butyl acetate has a very low potential to form tropospheric ozone (smog). Product and smog chamber studies⁵ have shown that tert-butyl acetate oxidizes to acetic anhydride (50%), acetone (20%), and organic nitrates (17-20%).

The maximum incremental reactivity (MIR) for tert-butyl acetate ranges between 40% and 70% of that of ethane and thereby meets the EPA's published criterion for "negligible photochemical reactivity."⁶

Ozone Depleting Potential – Tert-butyl acetate does not contain halogens and cannot, therefore, contribute to stratospheric ozone depletion. The USEPA has identified tert-butyl acetate and other esters as alternatives to ozone-depleting CFCs in solvent cleaning, aerosols, adhesives, coatings, and inks under the SNAP (Significant New Alternatives Policy).⁷

Acid Rain Forming Potential – Tert-butyl acetate also does not contain sulfur and cannot, therefore, form halo or sulfuric acids, two major contributors to acid rain formation. Since it does not contain nitrogen, its maximum potential to form nitric acid is limited to the ~20% yield of organic nitrates formed in polluted atmospheres.

Acetic anhydride, tert-butyl acetate's principal atmospheric product, will hydrolyze to acetic acid and be washed out. Compared to nitric, halo, and sulfuric acids, acetic acid is a very weak acid and will not contribute appreciably to acid rain formation.

*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).

Aquatic Fate

Volatilization – Most of the tert-butyl acetate released to water will volatilize within days and the rest will biodegrade within weeks. Based on a functional group estimation method, the Henry's Law Constant for tert-butyl acetate is calculated to be 3.3×10^{-6} atm•m³/mole at 25°C. This value of Henry's Law constant suggests that volatilization from environmental bodies of water will be rapid.¹

The volatilization half-life from a river one meter deep flowing 1 m/sec with a wind velocity of 3 m/sec is estimated to be 6.0 hours; the volatilization half-life from a similar river 10 meters deep is estimated to be 7.4 days.

Hydrolysis – The hydrolysis half-lives of tert-butyl acetate at pHs 7.0, 8.0, and 9.0 are about 135 years, 14.6 years, and 1.46 years, respectively, at 25°C. This indicates that hydrolysis will be important only in extremely alkaline environmental waters with pH values approaching 10 or higher.

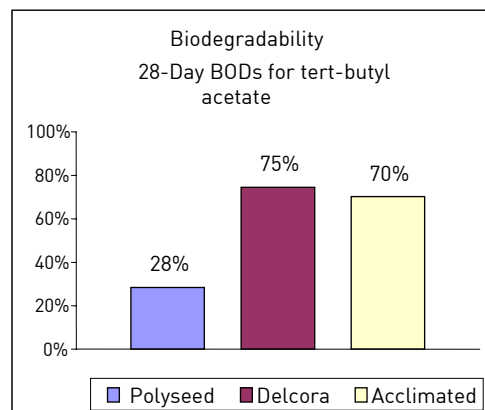
Biodegradation – Tert-butyl acetate has been shown⁸ to biodegrade in standard closed-bottle laboratory tests using acclimated and non-acclimated microorganisms. 28-day biological oxygen demand (BOD) expressed as % of chemical oxygen demand (COD) ranged from 28% with EPA-approved Polyseed to 75% with acclimated Delcora sludge typically found in Publicly-Owned Treatment Works (POTW) (see chart).

Chemicals with BOD greater than 60% of their COD are generally considered to be "readily biodegradable". Tert-butyl acetate is, therefore, either readily or inherently biodegradable, depending on the microorganisms present.

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Bioconcentration - Based on a log Kow (octanol-water coefficient) of 1.38, the bio-concentration factor (BCF) for tert-butyl acetate can be estimated to be 6.6 by an EPA-recommended regression-derived equation. This BCF value suggests that tert-butyl acetate bio-concentration is not significant.¹

Terrestrial Fate

Volatilization - Based on its high vapor pressure, tert-butyl acetate will evaporate relatively rapidly from wet or dry solid surfaces.¹

Leaching - Residual tert-butyl acetate in moist soil will rapidly migrate to bodies of water. Based on a log Kow (octanol-water coefficient) of 1.38, the Koc value for tert-butyl acetate can be estimated to be 134 by a regression-derived equation. This Koc value indicates high soil mobility.¹

Hydrolysis - Chemical hydrolysis of tert-butyl acetate in moist, very alkaline soils (pH 10 or higher) may be important, but hydrolysis in soils of pH 9 or lower will not occur to any appreciable extent.¹

References

¹Hazardous Substances Data Bank, Issue 98-2 (May 1998), U.S. National Library of Medicine.

²Letter from Spyros Pandis, Elias Associate Professor of Chemical Engineering, Carnegie Mellon University, September 1998.

³Don Wuebbles, Director Environmental Council, University of Illinois, Urbana-Champaign, Personal Communication, September 1998

⁴Reba Rubinstein, EPA SNAP staff, personal communication, 08/24/98.

⁵Tuazon, E. C.; Aschmann, S. M.; Atkinson, R.; Carter, W. P. L., J. Phys. Chem. A (1998), 102(13), 2316-2321.

⁶EPA-453/R-94-066-A, March 1995 Report to Congress, p. 3-5, footnote 2.

⁷40 CFR Parts 9 and 82, Protection of Stratospheric Ozone; Final Rule, Federal Register, Vol.59, No. 53

⁸Unpublished report, Raytheon Environmental Services Laboratory, August 1998.

This information is believed to be accurate as of the date of publication. It is the sole responsibility of the customer to determine whether the product is appropriate and suitable for the customer's specific use. Specific end uses may require approval by appropriate regulatory agencies. Lyondell Chemical Company makes no warranties, express or implied, regarding the product or information contained therein. The applicable Material Safety Data Sheet should be reviewed by customer before handling the Lyondell Chemical product. Lyondell Chemical Company disclaims any liability for infringement of any patent by reason of customer's use of any Lyondell Chemical Company products in combination with other materials or in any process.

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