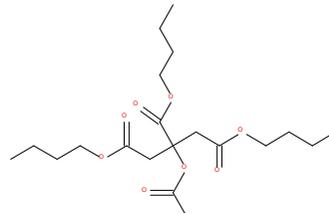




Acetyltributyl-citrate

Acetyltributyl citrate is used as a plasticizer, e.g. in PVC films. It is also used as a film former in nail polishes and creams.

Molar mass:
402.479 g/mol
CAS: 77-90-7
C₂₀H₃₄O₈



The measurements of the LANUV meet the following necessary criteria for clear identification:

- 1) Match of the exact mass, ± 5 ppm
- 2) Match of the isotope pattern, min. 70 %
- 3) Match of a reference spectrum
- 4) Match of the retention time with the reference substance

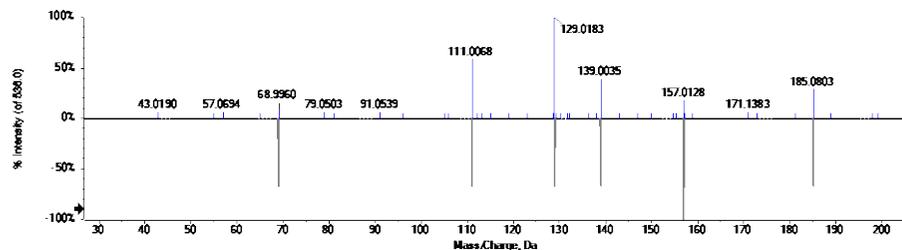


Figure 1: comparison of fragment-ion-spectra, blue: sample Wupper Opladen, grey: reference substance

Analytics and occurrence

Acetyltributyl citrate can be detected in positive mode with the existing measuring method. It was detected with different intensity in almost all investigated surface waters (Rhine, Ruhr, Wupper) and is therefore an ubiquitous substance. In some surface waters the general prevention value of 0.1 µg/L is exceeded.

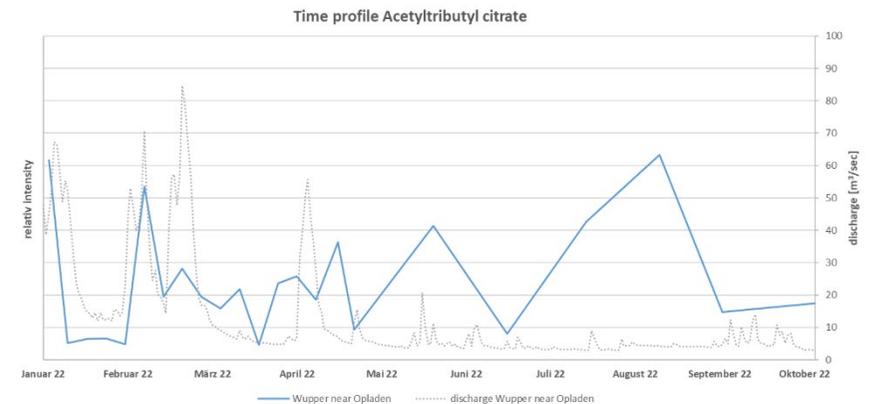


Figure 2: Time profile of Acetyltributyl citrate Wupper near Opladen

Relevance

For Acetyltributyl citrate there are no legally binding limit values for drinking water. Therefore, the general prevention value of 0.1 µg/L for drinking water is used for the assessment. Due to its (modeled) substance properties (high



sorption to soil particles, low mobility, biodegradable^{1,2}), the compound is not classified as potentially relevant to drinking water based on the data available to date. So far, no data are available for Acetyltributyl citrate on its behavior in drinking water treatment.

Data for Acetyltributyl citrate are available in the database of the European Chemicals Agency ECHA. Acute endpoints are given for three trophic levels (algae, daphnia, fish) and chronic data for algae and daphnia. The lowest chronic results for algae and daphnia are in the range between 0.1 - 1.1 mg/L. In some cases, the results vary significantly without any explanation in the literature. Therefore, the PNEC (Predicted No Effect Concentration) listed in the ECHA database was not adopted. The data listed in the ECHA database¹ indicate Acetyltributyl citrate as biodegradable. Modeled bioaccumulation factors indicate a low bioaccumulation potential.

Acetyltributyl citrate is not classified as a hazardous substance under EU Regulation 1272/2008 (CLP Regulation)³. An acceptable daily intake of 1 mg/kg bw/d was derived by the European Food Safety Authority (EFSA) in 2005⁴.

Further procedure:

Although Acetyltributyl citrate is ubiquitous and occurs regularly in comparable concentrations and exceeds the general prevention value of 0.1 µg/L in some waters, the substance is not included in the regular monitoring. By further measurements, no gain in knowledge is expected.

¹ ECHA – registration dossier, <https://echa.europa.eu/de/registration-dossier/-/registered-dossier/13143/5/3/1>
(Abruf: 17.05.2022)

² http://www.chemspider.com/Chemical-Structure.6259.html?rid=c4721703-ebbe-44a6-af4c-52d255679290&page_num=0 (Abruf: 17.05.2022)

³ ECHA (2022), C&L-Inventory Database, Tributyl O-acetylcitrate, <https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/111970> (Abruf: 20.05.2022)

⁴ EFSA (2005), Opinion of the Scientific Panel on food additives, flavourings, processing aids and materials in contact with food (AFC) on a request related to a 10th list of substances for food contact materials, The EFSA Journal (2005) 273, p 21 of 26, <https://efsa.onlinelibrary.wiley.com/doi/pdf/10.2903/j.efsa.2005.273a>