



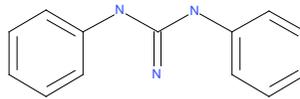
1,3- Diphenylguanidine

1,3-Diphenylguanidine (DPG) is a chemical used in rubber production as a vulcanization accelerator, mainly in tire production and in the manufacture of rubber soles.

Molare mass:
211.262 g/mol

CAS:
102-06-7

$C_{13}H_{13}N_3$



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

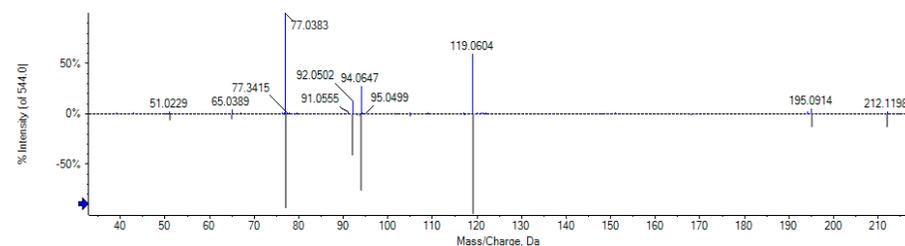


Figure 1: comparison of fragment-ion-spectra, blue: sample Wupper Opladen, grey: reference substance

Analytics and occurrence

1,3-Diphenylguanidine can be detected in positive mode with the existing measuring method. It was detected with different intensity in almost all investigated water bodies (Rhine, Ruhr, Wupper) and is therefore an ubiquitous substance. In some surface waters the general prevention value of $0.1 \mu\text{g/L}$ is exceeded. The concentrations range between 0.02 and $0.2 \mu\text{g/L}$.

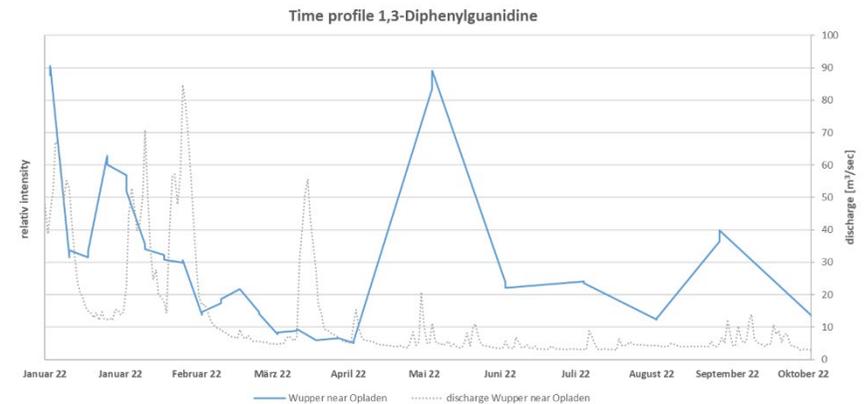


Figure 2: Time profile of 1,3-Diphenylguanidine Wupper near Opladen

Relevance

For 1,3-diphenylguanidine there are no legally binding limit values for drinking water. Therefore, the general prevention value of $0.1 \mu\text{g/L}$ for drinking water is used for the assessment. Due to its substance properties (polar, mobile, fate in the water phase, low bioaccumulation potential,



wide use in the EU¹), the substance is to be classified as potentially relevant to drinking water based on the data available to date.

1,3-Diphenylguanidine is considered to be highly biodegradable² in aerobic bank filtration passage. Due to its polarity, the removability of 1,3-diphenylguanidine should be evaluated for further drinking water treatment processes.

For 1,3-diphenylguanidine a report of the European Chemicals Agency ECHA from 2020 is available. In this report, a PNEC (Predicted No Effect Concentration) of 30 µg/L is deduced on the basis of a complete ecotoxicological data set for three trophic levels (algae, daphnia, fish). The PNEC is based on the chronic result from an algae test (NOEC/No Observed Effect Concentration: 300 µg/L).

The skin allergen 1,3-diphenylguanidine is harmful or toxic if swallowed (Acute Tox. 3 H301, Acute Tox. 4 H302)^{3,4}, and possibly genotoxic⁵. In the REACH dossier, the substance is classified by operators as probably toxic to reproduction based on a new study (Repr. Cat. 1B, H360FD). For the oral pathway a DNEL (Derived No Effect Level) of 0.017 mg/kg bw/d was derived for the general population⁶.

Further procedure:

Although 1,3-diphenylguanidine 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 - Substance Evaluation Conclusion, <https://echa.europa.eu/documents/10162/4df27360-03aa-3c93-54f0-08f8366f42f3> (Abruf: 17.05.2022)

² „Persistente und mobile Substanzen – eine (neue) Herausforderung für die Wasserversorgung am Rhein?“, Jahresbericht der Arbeitsgemeinschaft Rhein-Wasserwerke e. V. 2020

³ ECHA (2022), CLP-Inventory Database, 1,3-diphenylguanidine, <https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/91360> (Abruf: 19.05.2022)

⁴ ECHA (2022), Registry of CLH intentions until outcome, 1,3-diphenylguanidine, <https://echa.europa.eu/de/registry-of-clh-intentions-until-outcome/-/dislist/details/0b0236e183a4dc69> (Stand 24.01.2022)

⁵ HBM4EU (2020), Scoping document on Anilines, https://www.hbm4eu.eu/wp-content/uploads/2019/03/HBM4EU_D4.9_Scoping_Documents_HBM4EU_priority_substances_v1.0-Anilines.pdf (Stand Mai 2020)

⁶ ECHA (2021), REACH-Dossier, 1,3-diphenylguanidine, <https://echa.europa.eu/de/registration-dossier/-/registered-dossier/14992/1/2> (Stand 30.09.2021)