Non Target – News
#25

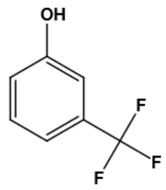
Landesamt für Natur,
Umwelt und Klima
Nordrhein-Westfalen

3-(Trifluoromethyl)phenol

Molar Mass:
162.11 g/mol

CAS: 98-17-9

$C_7H_5F_3O$



3-(trifluoromethyl)phenol, also known as 3-hydroxybenzotrifluoride or α,α,α-triflouro-m-cresol, is used as an intermediate in the manufacture of various chemical compounds, e.g. pesticides.[1] It is registered under the REACH Regulation, manufactured and/or imported into the European Economic Area, and used in industrial facilities. [2]

The measurements of the LANUK 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 with a reference spectrum
4) Match of the retention time with the reference substance

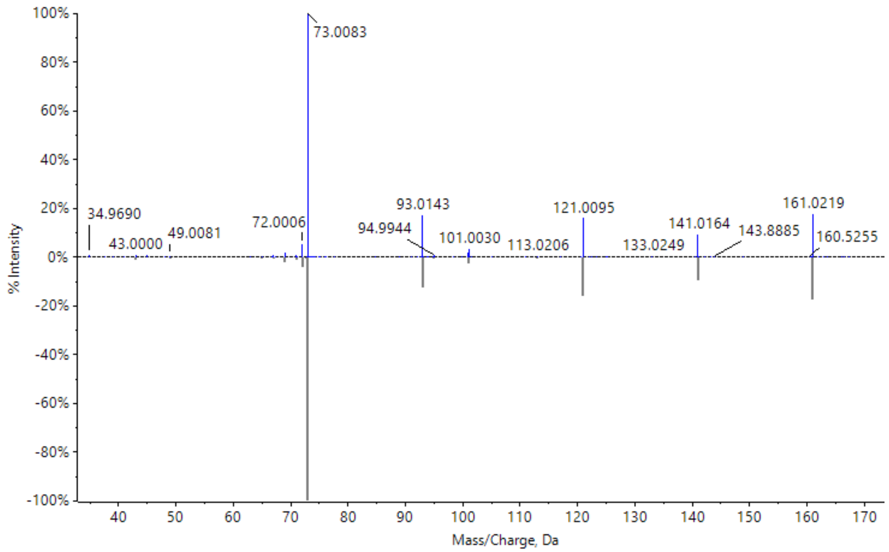


Figure 1: Comparison of fragment ion spectra (ESI negative); blue: wastewater treatment plant effluent from industrial site; grey: reference substance

Analytics und occurrence

As part of a measurement programme, selected wastewater discharges in North Rhine-Westphalia are analysed for the sum parameter AOF (adsorbable organically bound fluorine) in addition to official monitoring. In May 2025, an elevated AOF of 0.83 mg/L was measured in the sewage treatment plant effluent of an industrial site located in the Cologne administrative district. The sample was also tested for 30 per- and poly-

[1] https://www.ottokemi.com/research-essentials-chemicals/3trifluoromethylphenol-99-t-1889.aspx; accessed on 3 November 2025

[2] https://echa.europa.eu/mt/brief-profile/-/briefprofile/100.002.405; accessed on 3 November 2025

fluorinated alkyl substances[3], with only perfluorobutyric acid (0.078 µg/L), perfluorobutane sulfonic acid (0.089 µg/L) and perfluoropentanoic acid (0.035 µg/L) were detected above the lower application limit of 0.025 µg/L. The PFAS detected therefore did not explain the high AOF concentration. As a result, the sample was examined using non-target screening (HPLC-HRMS), which detected an unknown mass with high intensity that could be clearly identified as 3-(trifluoromethyl)phenol by comparison with the reference substance. A concentration of 406 µg/L 3-(trifluoromethyl)phenol was measured in the wastewater sample from May 2025.

Relevance

For 3-(trifluoromethyl)phenol, only individual test results on ecotoxicological effects are available in the database of the European Chemicals Agency (ECHA). No ecotoxicological assessment can be made on the basis of this data, especially as results from chronic test systems are lacking.

Information from the ECHA database indicates that 3-(trifluoromethyl)phenol is not readily biodegradable. A high bioaccumulation potential is not to be expected.

There are no legally binding limit values for 3-(trifluoromethyl)phenol in drinking water. The general precautionary value of 0.1 µg/L is therefore used for the assessment of drinking water production as a protected resource.

The European Chemicals Agency (ECHA) database classifies the substance as not readily biodegradable. Further data on substance properties or behaviour in drinking water treatment are currently not available. Based on the possible formation of the drinking water-relevant substance trifluoroacetic acid (TFA, CAS No.: 76-05-1) through the presence of the C-CF3 group[4; 5], the substance 3-(trifluoromethyl)phenol is provisionally classified as potentially relevant to drinking water.

If the database on the substance's properties and environmental behaviour improves, the classification of the substance should be reviewed.

Further procedure:

The relevant water authorities were informed of our findings and the responsible district government was asked to inform the polluter of the results. The industrial site's sewage treatment plant effluent will continue to be sampled and investigated to clarify whether the discharge into the wastewater is continuous or intermittent.

[3] Scope of PFAS measured: https://www.lanuk.nrw.de/themen/themenuebergreifende-aufgaben/gefahrstoffe/pfas/analytik; accessed on 3 November 2025

[4] Umweltbundesamt (2021): Chemikalieneintrag in Gewässer vermindern – Trifluoracetat (TFA) als persistente und mobile Substanz mit vielen Quellen. https://www.umweltbundesamt.de/sites/default/files/medien/11850/publikationen/2021_hg_chemiekalieneintrag_bf_v2.pdf; accessed on 3 November 2025

[5] Evidence for the formation of trifluoroacetate from diflufenican (Source: The Danish Environmental Protection Agency: Geological Survey of Denmark and Greenland (2024): TriFluPest
Trifluoreddikesyre (TFA) fra pesticider. https://www2.mst.dk/Udgiv/publikationer/2024/12/978-87-7038-688-3.pdf; accessed on 3 November 2025)