

1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone

EC number: 436-710-6

CAS number: 756-13-8

REACH



Classification & Labelling & PBT assessment

PBT assessment

S-01 | PBT assessment Summary

Administrative data

PBT assessment: overall result

PBT status:	the substance is not PBT / vPvB
Justification:	In accordance with screening criteria for persistence in Guidance document on information requirements and chemical safety assessment, chapter R.11: PBT Assessment (ECHA, 2017), the submission substance is not P/vP substance. In accordance with screening criteria for bioaccumulation in Guidance document on information requirements and chemical safety assessment, chapter R.11: PBT Assessment (ECHA, 2017), the submission substance is not B/vB substance. In accordance with criteria for toxicity in Guidance document on information requirements and chemical safety assessment, chapter R.11: PBT Assessment (ECHA, 2017), no conclusion on T can be reached. Therefore, the substance is not PBT/vPvB substance.

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EC number: 436-710-6 ; CAS number: 756-13-8



Environmental fate & pathways

Endpoint summary

S-01 | Environmental fate and pathways Summary

Administrative data

Description of key information

Additional information

Abiotic degradation:

The half-life of the substance under all test conditions (pH 1.2-9; temperature 25 and 37°C) is shorter than 2.5 minutes.

Biodegradation:

The PFPA (degradation product) is not readily biodegradable. In the biodegradation test according to OECD 301 B, the substance showed 3% biodegradation after 28 days in the test conditions.

Bioaccumulation and Geoaccumulation:

The predicted K_{oc} of the substance was 3904 L/kg with Log K_{oc} = 3.59 which indicated the potential for accumulation in soil.

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EC number: 436-710-6 · CAS number: 756-13-8



Ecotoxicological information

Ecotoxicological Summary

S-01 | Ecotoxicological information Summary (PNECs)

Administrative data

Hazard for aquatic organisms

Freshwater

Hazard assessment conclusion: PNEC aqua (freshwater)

PNEC value: 6.78 µg/L

Assessment factor: 1 000

Extrapolation method: assessment factor

PNEC freshwater (intermittent releases): 67.8 µg/L

Marine water

Hazard assessment conclusion: PNEC aqua (marine water)

PNEC value: 0.678 µg/L

Assessment factor: 10 000

Extrapolation method: assessment factor

STP

Hazard assessment conclusion: PNEC STP

PNEC value: 1 mg/L

Assessment factor: 100

Extrapolation method: assessment factor

Sediment (freshwater)

Hazard assessment conclusion: PNEC sediment (freshwater)

PNEC value: 2.67 mg/kg sediment dw

Extrapolation method: equilibrium partitioning method

Sediment (marine water)

Hazard assessment conclusion: PNEC sediment (marine water)

PNEC value: 0.267 mg/kg sediment dw

Extrapolation method: equilibrium partitioning method

Hazard for air

Air

Hazard assessment conclusion: no hazard identified

Hazard for terrestrial organisms

Soil

Hazard assessment conclusion: PNEC soil

PNEC value: 0.53 mg/kg soil dw

Extrapolation method: equilibrium partitioning method

Hazard for predators

Secondary poisoning

Hazard assessment conclusion: no potential for bioaccumulation

Additional information

The PNECs aqua were derived from the most sensitive test for the aquatic compartment, the short-term toxicity to algae. For other compartments, the PNECs are based on equilibrium partitioning.

Conclusion on classification

The short-term LC50 or EC50 values are >1070 mg/L for fish, > 1080 mg/L for daphnia and > 6.78 mg/L for algae.

In addition, the substance is not readily biodegradable, and has a log Kow of 2.79.

According to CLP (Directive 1272/2008/EC), the aquatic hazard of substance is classified as Chronic Category 2.

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REACH



Toxicological information

Toxicological Summary

S-01 | Toxicological information Summary (DN(M)ELs)

Administrative data

Workers - Hazard via inhalation route

Systemic effects

Long term exposure

Hazard assessment conclusion: DNEL (Derived No Effect Level)

Value: 83.4 mg/m³

Most sensitive endpoint: repeated dose toxicity

Route of original study: By inhalation

DNEL related information

DNEL derivation method: ECHA REACH Guidance

Overall assessment factor (AF): 75

Dose descriptor starting point: NOAEC

Value: 12 450 mg/m³

Modified dose descriptor starting point: NOAEC

Value: 6 260 mg/m³

Explanation for the modification of the dose descriptor starting point: Default (DNEL calculator)

AF for dose response relationship: 1

Justification: Default (DNEL calculator)

AF for differences in duration of exposure: 6

Justification: Default (DNEL calculator)

AF for interspecies differences (allometric scaling): 1

Justification: Default (DNEL calculator)

AF for other interspecies differences: 2.5

Justification: Default (DNEL calculator)

AF for intraspecies differences: 5

Justification: Default (DNEL calculator)

AF for the quality of the whole database: 1

Justification: Default (DNEL calculator)

Acute/short term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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DNEL related information

Local effects

Long term exposure

Hazard assessment conclusion:	no hazard identified
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Acute/short term exposure

Hazard assessment conclusion:	no hazard identified
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DNEL related information

Workers - Hazard via dermal route

Systemic effects

Long term exposure

Hazard assessment conclusion:	DNEL (Derived No Effect Level)
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Value:	11.8 mg/kg bw/day
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Most sensitive endpoint:	repeated dose toxicity
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Route of original study:	By inhalation
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DNEL related information

DNEL derivation method:	ECHA REACH Guidance
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Overall assessment factor (AF):	300
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Dose descriptor starting point:	NOAEC
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Value:	12 450 mg/m ³
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Value:	3 550 mg/kg bw/day
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Explanation for the modification of the dose descriptor starting point:	Default (DNEL calculator)
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AF for dose response relationship:	1
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Justification:	Default (DNEL calculator)
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AF for differences in duration of exposure:	6
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Justification:	Default (DNEL calculator)
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AF for interspecies differences (allometric scaling):	4
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Justification:	Default (DNEL calculator)
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AF for other interspecies differences:	2.5
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Justification:	Default (DNEL calculator)
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AF for intraspecies differences:	5
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Justification:	Default (DNEL calculator)
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AF for the quality of the whole database:	1
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Justification:	Default (DNEL calculator)
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Acute/short term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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DNEL related information

Local effects

Long term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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Acute/short term exposure

Hazard assessment conclusion:	no hazard identified
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Workers - Hazard for the eyes

Local effects

Hazard assessment conclusion:	no hazard identified
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Additional information - workers

General Population - Hazard via inhalation route

Systemic effects

Long term exposure

Hazard assessment conclusion:	DNEL (Derived No Effect Level)
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Value:	14.8 mg/m ³
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Most sensitive endpoint:	repeated dose toxicity
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Route of original study:	By inhalation
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DNEL related information

DNEL derivation method:	ECHA REACH Guidance
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Overall assessment factor (AF):	150
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Dose descriptor starting point:	NOAEC
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Value:	12 450 mg/m ³
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Value:	2 220 mg/m ³
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Explanation for the modification of the dose descriptor starting point:	Default (DNEL calculator)
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AF for dose response relationship:	1
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Justification:	Default (DNEL calculator)
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AF for differences in duration of exposure:	6
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Justification:	Default (DNEL calculator)
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AF for interspecies differences (allometric scaling):	1
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Justification:	Default (DNEL calculator)
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AF for other interspecies differences:	2.5
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Justification:	Default (DNEL calculator)
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AF for intraspecies differences:	10
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Justification:	Default (DNEL calculator)
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AF for the quality of the whole database:	1
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Justification:	Default (DNEL calculator)
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Acute/short term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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DNEL related information

Local effects

Long term exposure

Hazard assessment conclusion:	no hazard identified
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Acute/short term exposure

Hazard assessment conclusion:	no hazard identified
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DNEL related information

General Population - Hazard via dermal route

Systemic effects

Long term exposure

Hazard assessment conclusion:	DNEL (Derived No Effect Level)
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Value:	4.26 mg/kg bw/day
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Most sensitive endpoint:	repeated dose toxicity
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Route of original study:	By inhalation
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DNEL related information

DNEL derivation method:	ECHA REACH Guidance
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Overall assessment factor (AF):	600
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Dose descriptor starting point:	NOAEC
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Value:	12 450 mg/m ³
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Value:	2 560 mg/kg bw/day
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Explanation for the modification of the dose descriptor starting point:	Default (DNEL calculator)
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AF for dose response relationship:	1
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Justification:	Default (DNEL calculator)
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AF for differences in duration of exposure:	6
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Justification:	Default (DNEL calculator)
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AF for interspecies differences (allometric scaling):	4
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Justification:	Default (DNEL calculator)
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AF for other interspecies differences:	2.5
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Justification:	Default (DNEL calculator)
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AF for intraspecies differences:	10
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Justification:	Default (DNEL calculator)
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AF for the quality of the whole database:	1
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Justification:	Default (DNEL calculator)
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Acute/short term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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DNEL related information

Local effects

Long term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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Acute/short term exposure

Hazard assessment conclusion:	no hazard identified
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General Population - Hazard via oral route

Systemic effects

Long term exposure

Hazard assessment conclusion:	DNEL (Derived No Effect Level)
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Value:	4.26 mg/kg bw/day
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Most sensitive endpoint:	repeated dose toxicity
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Route of original study:	By inhalation
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DNEL related information

DNEL derivation method:	ECHA REACH Guidance
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Overall assessment factor (AF):	600
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Dose descriptor starting point:	NOAEC
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Value:	12 450 mg/kg bw/day
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Modified dose descriptor starting point:	NOAEL
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Value:	2 560 mg/kg bw/day
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Explanation for the modification of the dose descriptor starting point:	Default (DNEL calculator)
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AF for dose response relationship:	1
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Justification:	Default (DNEL calculator)
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AF for differences in duration of exposure:	6
---	---

Justification:	Default (DNEL calculator)
----------------	---------------------------

AF for interspecies differences (allometric scaling):	4
---	---

Justification:	Default (DNEL calculator)
----------------	---------------------------

AF for other interspecies differences:	2.5
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Justification:	Default (DNEL calculator)
----------------	---------------------------

AF for intraspecies differences:	10
----------------------------------	----

Justification:	Default (DNEL calculator)
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AF for the quality of the whole database:	1
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Justification:	Default (DNEL calculator)
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Acute/short term exposure

Hazard assessment conclusion:	hazard unknown but no further hazard information necessary as no exposure expected
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DNEL related information

General Population - Hazard for the eyes

Local effects

no hazard identified

Additional information - General Population

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