

# 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: | <p>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.</p> <p>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.</p> <p>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.</p> <p>Therefore, the substance is not PBT/vPvB substance.</p> |

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

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<sub>oc</sub> of the substance was 3904 L/kg with Log K<sub>oc</sub> = 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

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### Air

Hazard assessment conclusion: no hazard identified

## Hazard for terrestrial organisms

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### 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

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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

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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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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/m<sup>3</sup>

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/m<sup>3</sup>

Modified dose descriptor starting point: NOAEC

Value: 6 260 mg/m<sup>3</sup>

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 |
|-------------------------------|------------------------------------------------------------------------------------|

#### DNEL related information

#### Local effects

##### Long term exposure

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

#### Acute/short term exposure

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

#### DNEL related information

### Workers - Hazard via dermal route

#### Systemic effects

##### Long term exposure

|                               |                                |
|-------------------------------|--------------------------------|
| Hazard assessment conclusion: | DNEL (Derived No Effect Level) |
|-------------------------------|--------------------------------|

|        |                   |
|--------|-------------------|
| Value: | 11.8 mg/kg bw/day |
|--------|-------------------|

|                          |                        |
|--------------------------|------------------------|
| 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): | 300 |
|---------------------------------|-----|

|                                 |       |
|---------------------------------|-------|
| Dose descriptor starting point: | NOAEC |
|---------------------------------|-------|

|        |                          |
|--------|--------------------------|
| Value: | 12 450 mg/m <sup>3</sup> |
|--------|--------------------------|

|        |                    |
|--------|--------------------|
| Value: | 3 550 mg/kg bw/day |
|--------|--------------------|

|                                                                         |                           |
|-------------------------------------------------------------------------|---------------------------|
| 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): | 4 |
|-------------------------------------------------------|---|

|                |                           |
|----------------|---------------------------|
| 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 |
|-------------------------------|------------------------------------------------------------------------------------|

#### DNEL related information

## Local effects

### Long term exposure

|                               |                                                                                    |
|-------------------------------|------------------------------------------------------------------------------------|
| Hazard assessment conclusion: | hazard unknown but no further hazard information necessary as no exposure expected |
|-------------------------------|------------------------------------------------------------------------------------|

### Acute/short term exposure

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

## Workers - Hazard for the eyes

### Local effects

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

## Additional information - workers

## General Population - Hazard via inhalation route

### Systemic effects

#### Long term exposure

|                               |                                |
|-------------------------------|--------------------------------|
| Hazard assessment conclusion: | DNEL (Derived No Effect Level) |
|-------------------------------|--------------------------------|

|        |                        |
|--------|------------------------|
| Value: | 14.8 mg/m <sup>3</sup> |
|--------|------------------------|

|                          |                        |
|--------------------------|------------------------|
| 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): | 150 |
|---------------------------------|-----|

|                                 |       |
|---------------------------------|-------|
| Dose descriptor starting point: | NOAEC |
|---------------------------------|-------|

|        |                          |
|--------|--------------------------|
| Value: | 12 450 mg/m <sup>3</sup> |
|--------|--------------------------|

|        |                         |
|--------|-------------------------|
| Value: | 2 220 mg/m <sup>3</sup> |
|--------|-------------------------|

|                                                                         |                           |
|-------------------------------------------------------------------------|---------------------------|
| 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: | 10 |
|----------------------------------|----|

|                |                           |
|----------------|---------------------------|
| 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 |
|-------------------------------|------------------------------------------------------------------------------------|

#### DNEL related information

#### Local effects

#### Long term exposure

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

#### Acute/short term exposure

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

#### DNEL related information

### General Population - Hazard via dermal route

#### Systemic effects

#### Long term exposure

|                               |                                |
|-------------------------------|--------------------------------|
| Hazard assessment conclusion: | DNEL (Derived No Effect Level) |
|-------------------------------|--------------------------------|

|        |                   |
|--------|-------------------|
| Value: | 4.26 mg/kg bw/day |
|--------|-------------------|

|                          |                        |
|--------------------------|------------------------|
| 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): | 600 |
|---------------------------------|-----|

|                                 |       |
|---------------------------------|-------|
| Dose descriptor starting point: | NOAEC |
|---------------------------------|-------|

|        |                          |
|--------|--------------------------|
| Value: | 12 450 mg/m <sup>3</sup> |
|--------|--------------------------|

|        |                    |
|--------|--------------------|
| Value: | 2 560 mg/kg bw/day |
|--------|--------------------|

|                                                                         |                           |
|-------------------------------------------------------------------------|---------------------------|
| 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): | 4 |
|-------------------------------------------------------|---|

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

|                                        |     |
|----------------------------------------|-----|
| AF for other interspecies differences: | 2.5 |
|----------------------------------------|-----|

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

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

|                |                           |
|----------------|---------------------------|
| 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 |
|-------------------------------|------------------------------------------------------------------------------------|

#### DNEL related information

## Local effects

### Long term exposure

|                               |                                                                                    |
|-------------------------------|------------------------------------------------------------------------------------|
| Hazard assessment conclusion: | hazard unknown but no further hazard information necessary as no exposure expected |
|-------------------------------|------------------------------------------------------------------------------------|

### Acute/short term exposure

|                               |                      |
|-------------------------------|----------------------|
| Hazard assessment conclusion: | no hazard identified |
|-------------------------------|----------------------|

## General Population - Hazard via oral route

### Systemic effects

#### Long term exposure

|                               |                                |
|-------------------------------|--------------------------------|
| Hazard assessment conclusion: | DNEL (Derived No Effect Level) |
|-------------------------------|--------------------------------|

|        |                   |
|--------|-------------------|
| Value: | 4.26 mg/kg bw/day |
|--------|-------------------|

|                          |                        |
|--------------------------|------------------------|
| 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): | 600 |
|---------------------------------|-----|

|                                 |       |
|---------------------------------|-------|
| Dose descriptor starting point: | NOAEC |
|---------------------------------|-------|

|        |                     |
|--------|---------------------|
| Value: | 12 450 mg/kg bw/day |
|--------|---------------------|

|                                          |       |
|------------------------------------------|-------|
| Modified dose descriptor starting point: | NOAEL |
|------------------------------------------|-------|

|        |                    |
|--------|--------------------|
| Value: | 2 560 mg/kg bw/day |
|--------|--------------------|

|                                                                         |                           |
|-------------------------------------------------------------------------|---------------------------|
| 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): | 4 |
|-------------------------------------------------------|---|

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

|                                        |     |
|----------------------------------------|-----|
| AF for other interspecies differences: | 2.5 |
|----------------------------------------|-----|

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

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

|                |                           |
|----------------|---------------------------|
| 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 |
|-------------------------------|------------------------------------------------------------------------------------|

#### DNEL related information

## General Population - Hazard for the eyes

### Local effects

no hazard identified

## Additional information - General Population

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