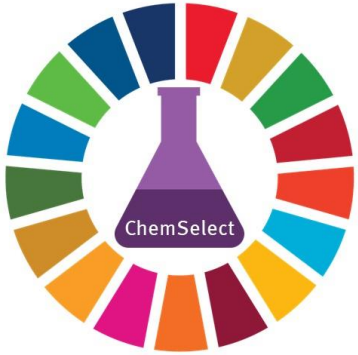
ChemSelect: Example Coolants



by

Antonia Reihlen,
Ökopol, Hamburg

Dirk Bunke
Ökoinstitut e.V., Freiburg

Editor:
German Environment Agency

Table of content

1 Introduction

ChemSelect is an online application that enables formulators and end users of chemicals to assess the sustainability of substances and mixtures. During its development, ChemSelect was tested by various people on many substances and mixtures. This also included comparisons between two products or more that are intended for the same use and differ in their composition. Some of these couples have been selected as examples. They are used in information materials about ChemSelect and also as training material. We use these reports to describe the examples. In these examples, the experiences gained during evaluating the example chemicals are also documented.

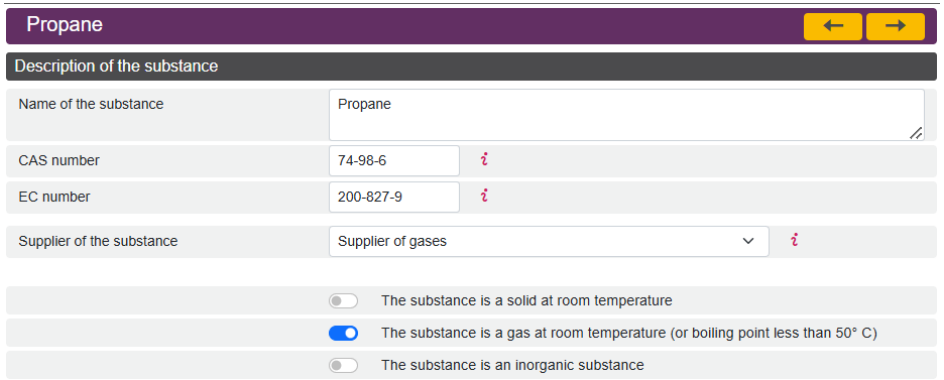
To understand the colour scheme: For each criterion, a colour and a number are assigned that indicate the degree of sustainability: Red/5 not sustainable; Green/1 = sustainable and yellow/3 = "in the middle". If information is missing, the rating is pink/4. If no entry has been made for a criterion, it is grey/-1. If a criterion is not relevant for a substance or use (e.g. persistent for inorganic substances), a light blue/-2 is assigned. Details on the sustainability indicators and the methodology for aggregating the sub-criteria into the main criteria can be found in the evaluation concept.

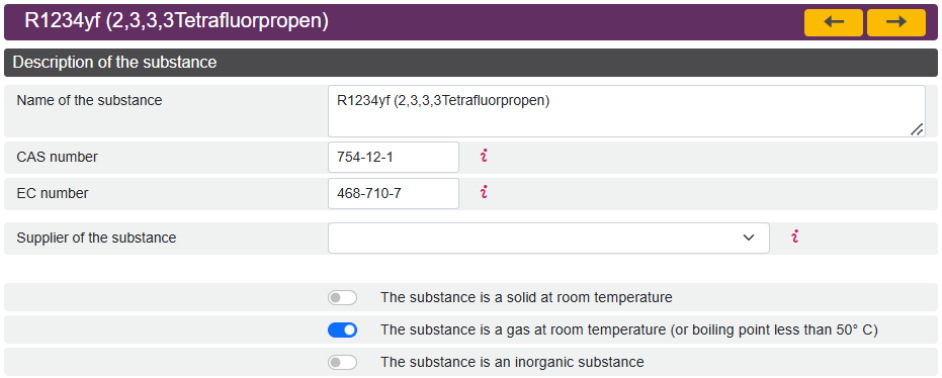
2 Background information about the products

2.1 Application area and functionality

The evaluated products are gases that are used as coolants, for example in air conditioning systems. Coolants are only handled by professional users; the air conditioning systems can be used commercially or privately. In this example it is assumed that the air conditioning systems containing the coolants are disposed of in Europe and that controlled removal of the coolants is therefore ensured. The evaluation was carried out by the user of the coolant.

2.2 Details about the products

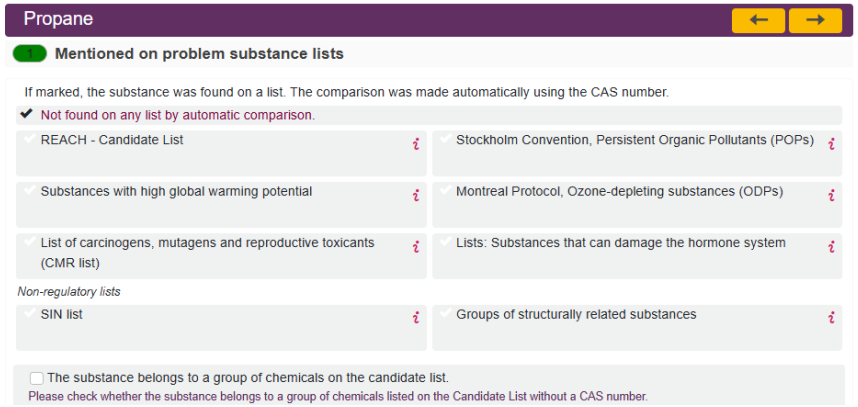


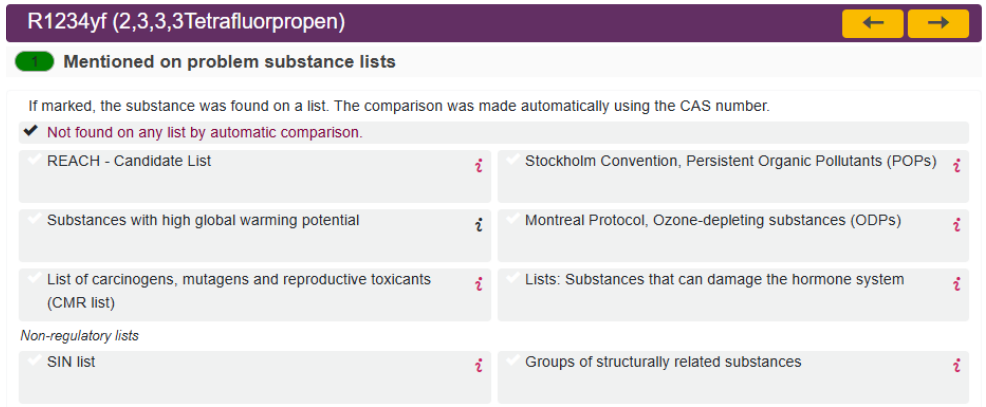


The two coolants are supplied by the same supplier. They are both gaseous, so the “slider” at the button is set to blue.

3 Assessment

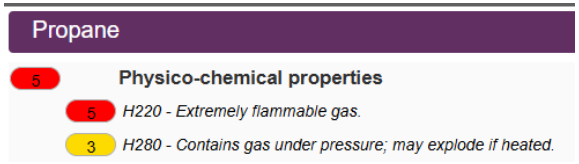
3.1 Lists of problematic substances

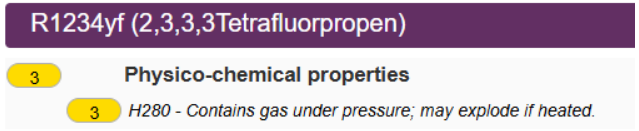




None of the two substances is included in a list of problematic substances

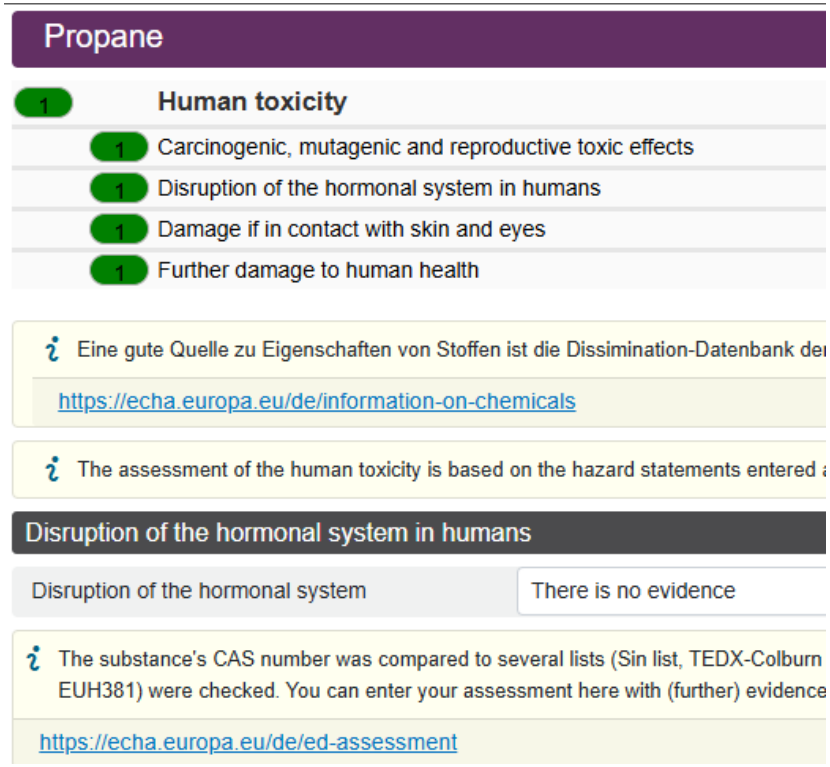
3.2 Physical-chemical properties

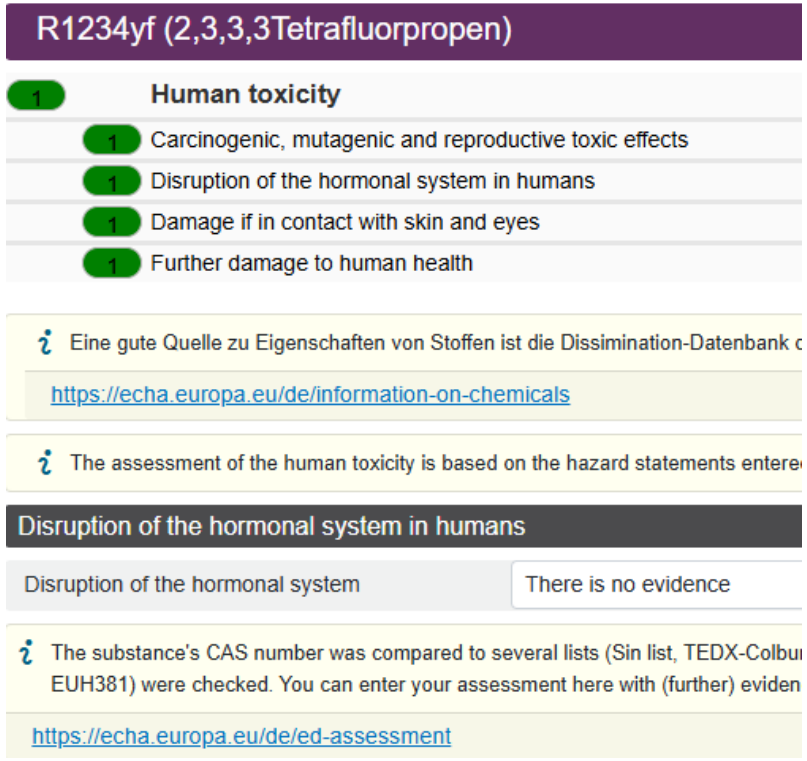




Both substances can explode when heated. Propane is also flammable. The evaluation is based on the H statements entered.

3.3 Human toxicity





Both gases are not harmful to humans. Respiratory problems are known for propane at very high inhaled concentrations; however, this does not lead to a classification. Therefore the results for both gases are identical.

R1234fy is broken down in the atmosphere into, among other things, trifluoroacetic acid (TFA) and is washed out of the air with rain. TFA is persistent and very mobile and reaches aquifers, some of which are used as a source of drinking water. The German authorities have submitted an application for a harmonized classification as toxic to reproduction. There is no option to enter information about classification proposals for carcinogenicity, mutagenicity and reprotoxic effects (CMR), but this information should be kept in mind and respective processes be watched.

If the breakdown product of R1234yf will be classified as reprotoxic, the assessment will result in a red mark for the CMR sub-criterion.

3.4 Environmental toxicity

In the evaluation of the environmental toxicity of R1234yf, its degradation to TFA can be taken into account as a category “suspected” or “indications in literature” exist. Although not yet manifesting in a harmonised classification, there are very strong indications of TFA being a PMT or vPvM. Therefore, the option that the literature (already) refers to TFA as a PMT is selected. Trifluoro acetic acid is also classified as H412. This H statement has been inserted for the substance R1234yf as the precursor of TFA.

The “Long-distance transport” parameter is set to “not relevant” as the default, since gases are and remain in the air. Their transport distance primarily depends on their persistence in air, which is considered already in the PBT/vPvB or PMT/vPvM criterion. Long-distance transport is therefore not included in the rating at all.

Propane

1 Environmental toxicity

- 1 Aquatic toxicity
- 1 PBT/vPvB substances and long-distance transport
- 1 PMT/vPvM substances
- 1 Disruptions of the hormone system in the environment

The assessment of the environmental toxicity is based on the hazard statements entered at the beginning. In addition, additional sources can be taken into account for various aspects.

☐ This is an inorganic substance

Aquatic toxicity

This criterion is used to access the acute and chronic toxicity to aquatic organisms.

Relevant H statements No

There is no classification for aquatic toxicity. Enter data from studies to assess the criterion.

Acute aquatic toxicity (LC50) [mg/l]	
Chronic aquatic toxicity (NOEC or EC10) [mg/l]	

PBT/vPvB substances and long-distance transport

PBT/vPvB

Information on PBT properties	No indication of PBT/ vPvB properties

PERSISTENCE
Simulation study: (not recorded) -- Days
Degradability: Not relevant
BIOACCUMULATION
Bioconcentration factor (BCF):
Octanol-water partition coefficient (LogKow):
TOXICITY
Chronic toxicity from studies: mg/l

Record measured values

Long-distance transport

Long-distance transport is not relevant for gaseous substances.

PMT/vPvM substances

This criterion assesses whether a substance can pose a risk to drinking water supplies due to its persistence (

Information about PMT/vPvM properties	No evidence of PMT/ vPvM properties

Disruptions of the hormone system in the environment

This indicator shows whether a substance can disrupt the hormone system of organisms in the environment.

Endocrine disrupting properties of the substance	No evidence of endocrine activity

R1234yf (2,3,3,3Tetrafluorpropen)

5 Environmental toxicity

- 3 Aquatic toxicity
- 1 PBT/vPvB substances and long-distance transport
- 5 PMT/vPvM substances
- 1 Disruptions of the hormone system in the environment

The assessment of the environmental toxicity is based on the hazard statements entered at the beginning. In addition, fu additional sources can be taken into account for various aspects.

☐ This is an inorganic substance

Aquatic toxicity

This criterion is used to access the acute and chronic toxicity to aquatic organisms.

Relevant H statements H412

The criterion is evaluated based on the classification. Entering additional information is possible but not required.

Acute aquatic toxicity (LC50) [mg/l]	
Chronic aquatic toxicity (NOEC or EC10) [mg/l]	100,00000

PBT/vPvB substances and long-distance transport

PBT/vPvB

Information on PBT properties	Own evaluation by entering measured values

PERSISTENCE
Simulation study: (not recorded) -- Days
Degradability: Not biodegradable
BIOACCUMULATION
Bioconcentration factor (BCF):
Octanol-water partition coefficient (LogKow): 2.00
TOXICITY
Chronic toxicity from studies: 100.0000000 mg/l

Record measured values

Long-distance transport

Long-distance transport is not relevant for gaseous substances.

PMT/vPvM substances

This criterion assesses whether a substance can pose a risk to drinking water supplies due to its persistence (P), its mobil

Information about PMT/vPvM properties	The substance is referred to in the literature as PMT/vPvM

Disruptions of the hormone system in the environment

This indicator shows whether a substance can disrupt the hormone system of organisms in the environment.

Endocrine disrupting properties of the substance	No evidence of endocrine activity

3.5 Exposure potential

Propane

1	Exposure potential for workers
-2	Exposure potential for consumers
1	Exposure potential for the environment

Even if the exposure potentials are yellow or green here, there may be situations with a very high exposure potential (red). Please, check the detailed results using the tab "evaluation".

Szenario for gas | Application quantities for gas | Evaluation

Results

Life cycle	Formulation	Application	Processing Product	Use Product	Waste treatment
Target					
Worker / Dermal	16	16	13	20	20
Worker / Inhalative	9	9	13	11	11
Consumer / Dermal		9		13	
Consumer / Inhalative		5		9	
Consumer / Orally		9		13	
Environment / Water	3	3	3	3	3
Environment / Air	5	5	5	5	5
Environment / Soil	3	3	3	3	3

R1234yf (2,3,3,3Tetrafluorpropen)

1	Exposure potential for workers
-2	Exposure potential for consumers
1	Exposure potential for the environment

Even if the exposure potentials are yellow or green here, there may be situations with a very high exposure potential (red). Please, check the detailed results using the tab "evaluation".

Szenario for gas | Application quantities for gas | Evaluation

Results

Life cycle	Formulation	Application	Processing Product	Use Product	Waste treatment
Target					
Worker / Dermal	16	16	13	20	20
Worker / Inhalative	9	9	13	11	11
Consumer / Dermal		9		13	
Consumer / Inhalative		5		9	
Consumer / Orally		9		13	
Environment / Water	4	4	4	4	4
Environment / Air	5	5	5	5	5
Environment / Soil	4	4	4	4	4

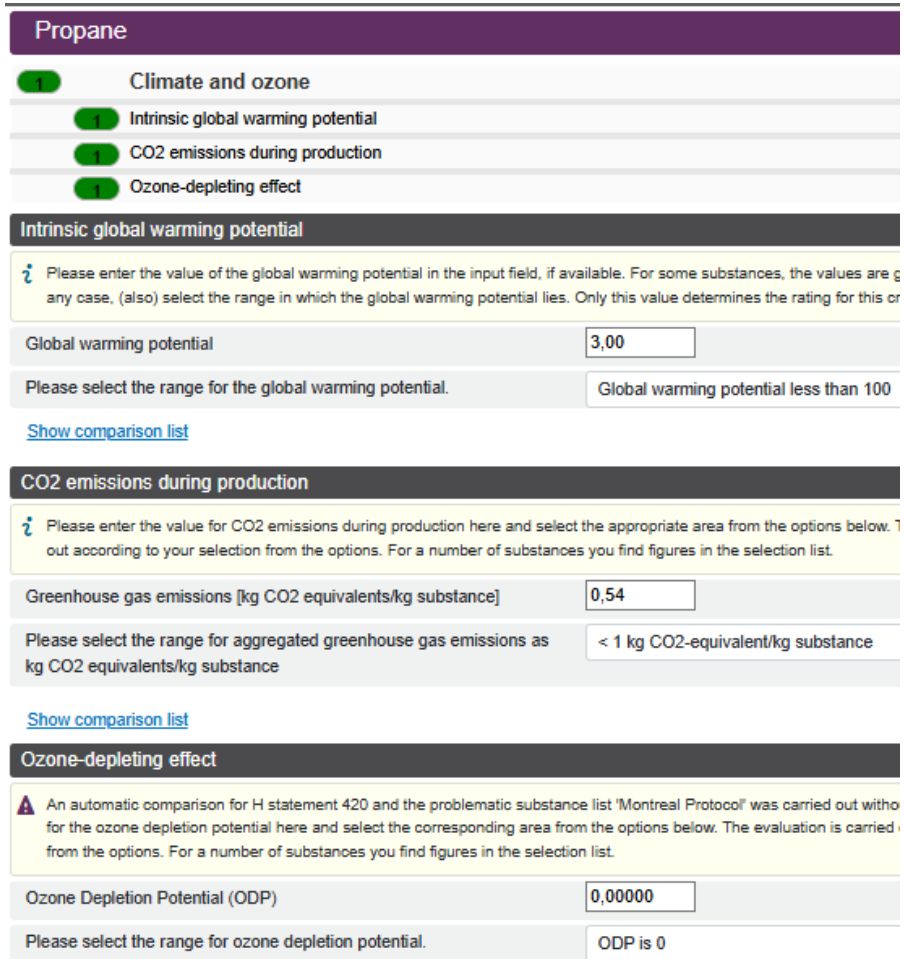
The two gases are used in the same application. Therefore, the use scenarios are also the same.

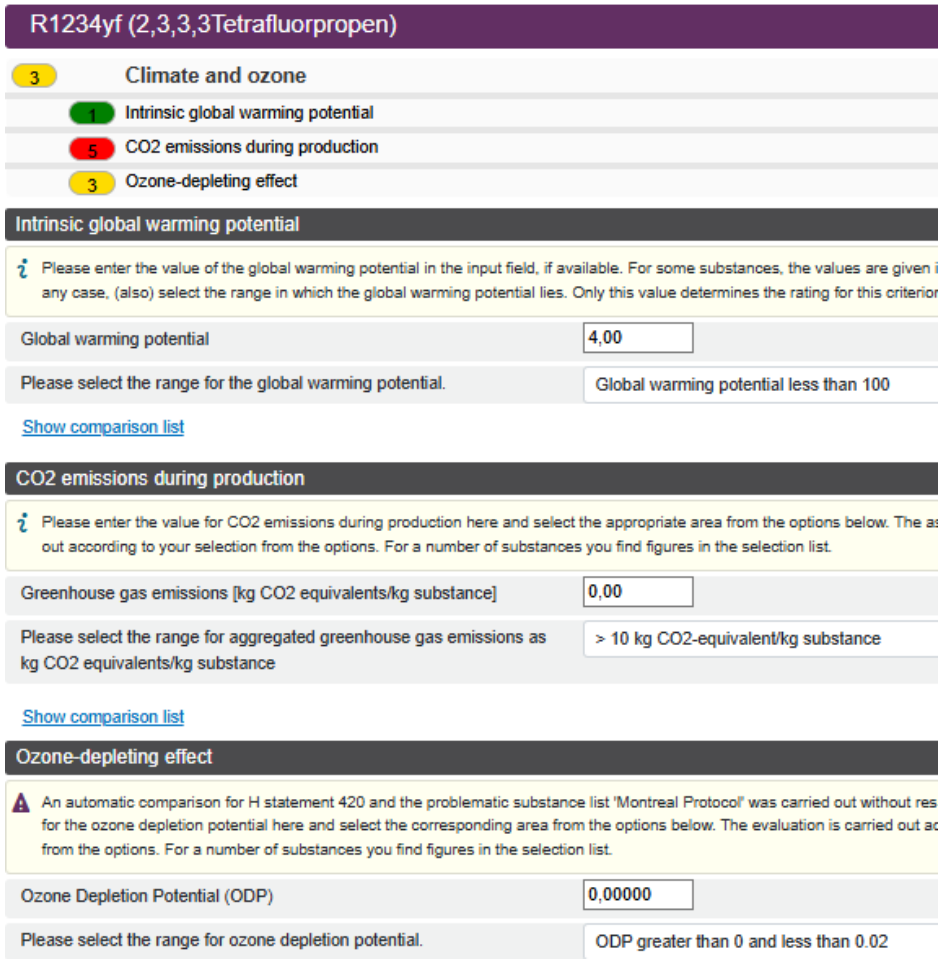
For gases, compared to non-gaseous substances and mixtures, the assessment of exposure potentials is modified because it is assumed that relevant releases occur at exactly one point in the life cycle. For the current product, this happens at the end of life of the air conditioning system. Air conditioning systems are disposed of in a controlled manner, at least in Europe, and the coolant is collected largely emission-free. Therefore, only low emissions are expected.

Both gases are used as pure gases, so the highest concentration ranges are entered.

Since only small releases of refrigerants are to be expected, the possible exposure of both employees and the environment is rated as “low”, i.e. green. Consumers do not normally come into contact with the coolants (blue colour).

3.6 Climate and ozone impacts



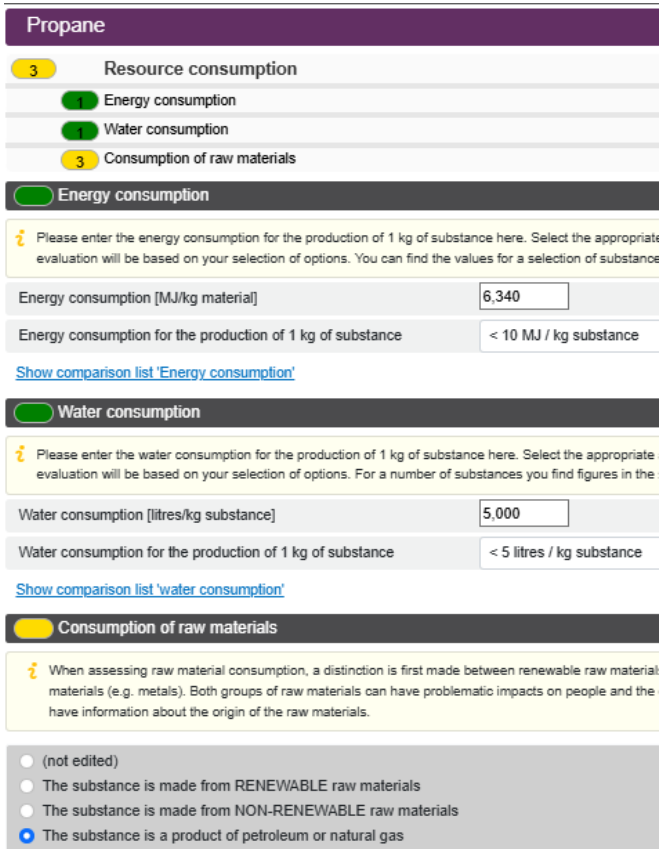


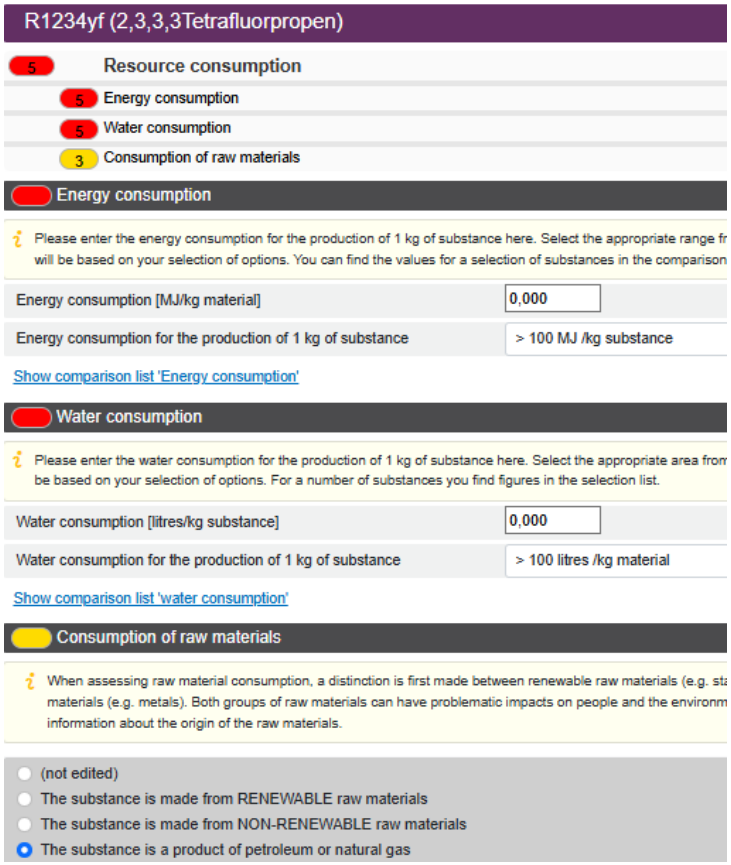
R1234yf is used as a replacement for very ozone-damaging coolants. It has a relatively low GWP. However, its production is energy-intensive, thus associated with high CO2 emissions (red). In addition, the production of R1234yf leads to the generation and emission of other ozone depleting

substances[1]. Therefore, the ODP is set to yellow, even though R1234yf itself is not ozone-depleting. Since no specific value was found for these emissions, only the range is selected.

Propane is a component of natural gas and can be obtained relatively inexpensively. It has a low GWP, relatively little energy (CO2 emissions) is used during production and it does not damage the ozone layer. Information on the lifecycle have been found on the internet.

3.7 Resource consumption

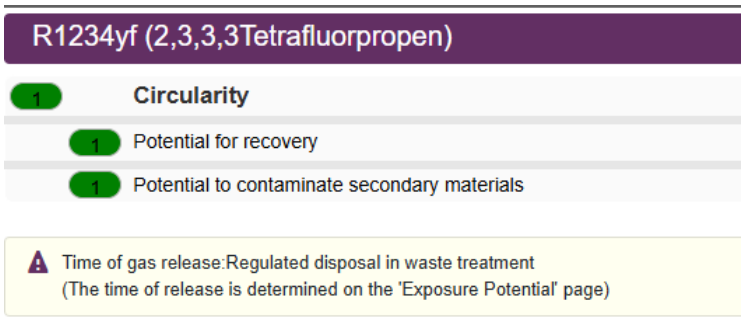




[1] https://www.autoklimaanlage.info/fileadmin/user_upload/pdfs/Faktenblatt_1234yf_270812.pdf

With the exception of hydrofluoric acid, all fluorine-containing substances are rated red in the comparison list for energy consumption. Therefore R1234yf is also rated red. With the exception of aluminium fluoride, all fluorine-containing compounds are rated red in the comparison list for water consumption. Therefore, the water consumption of R1234 is also rated red. Both ratings are set to green for propane, which is viewed more as a "base material". Here, information were available from a lifecycle inventory. Both compounds are made from petroleum or natural gas, so the assessment of raw material consumption does not differ.

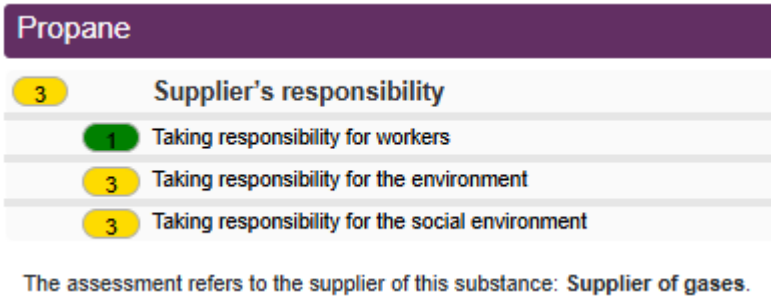
3.8 Circularity potential

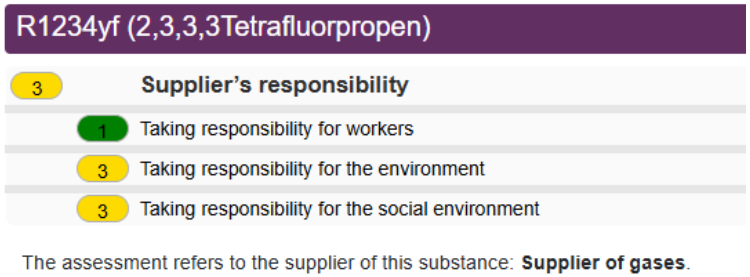


Both coolants can theoretically be recovered from the products in which they are used. Losses are possible along the lifetime from air conditioning systems but should be kept to a minimum (closed system). Contamination of the other components during the recycling stage is almost impossible due to the gaseous nature of the coolants. Therefore, the potential for recovery and the potential for contaminating secondary materials are both evaluated as green.

In Europe, products containing coolants are collected separately and sent for specific disposal. This may not be the case in other countries. It is up to the user whether this assessment should be changed as a result; the criterion only evaluates the potential, but not the actual disposal that takes place.

3.9 Supplier responsibility

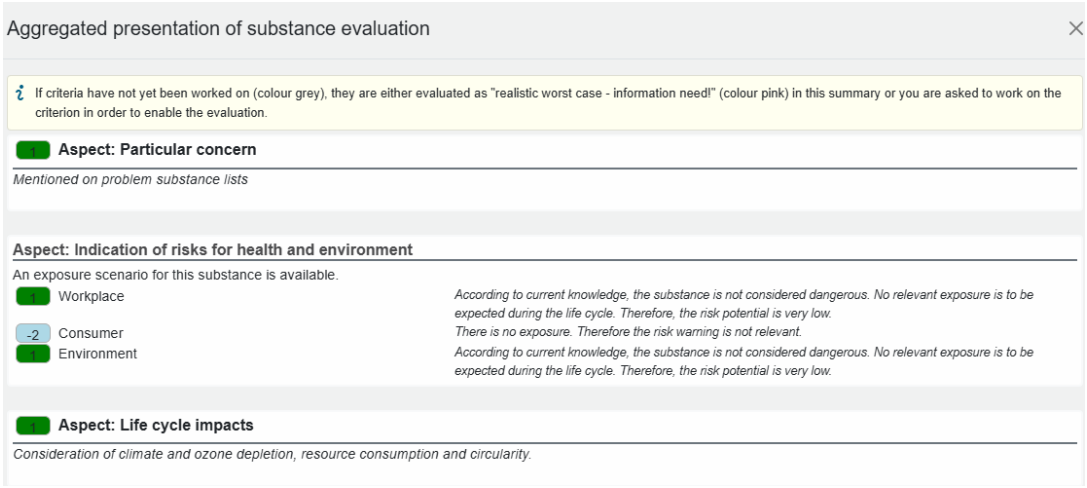




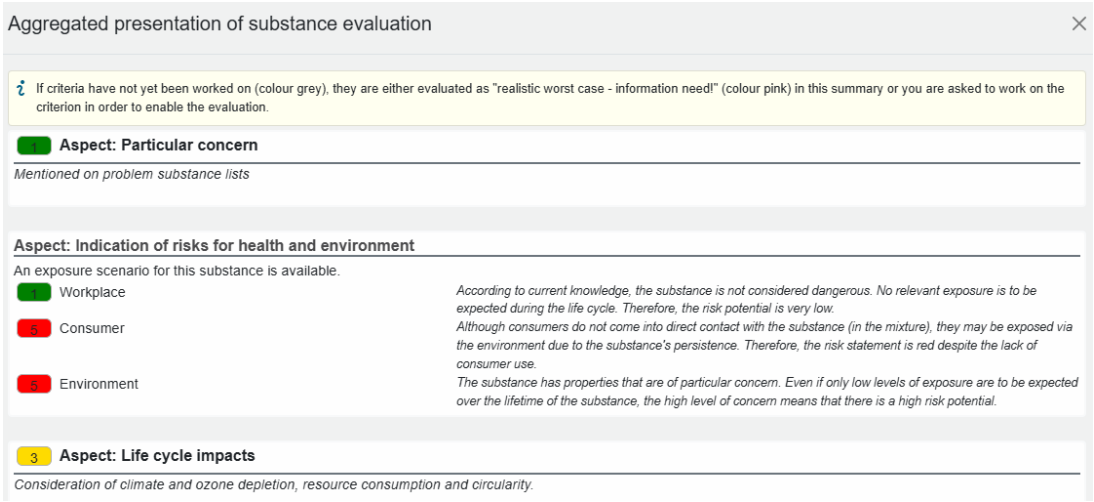
Since both gases are purchased from the same supplier, the evaluation does not differ. The supplier's rating is shown in the figure below.

3.10 Summary

Propane



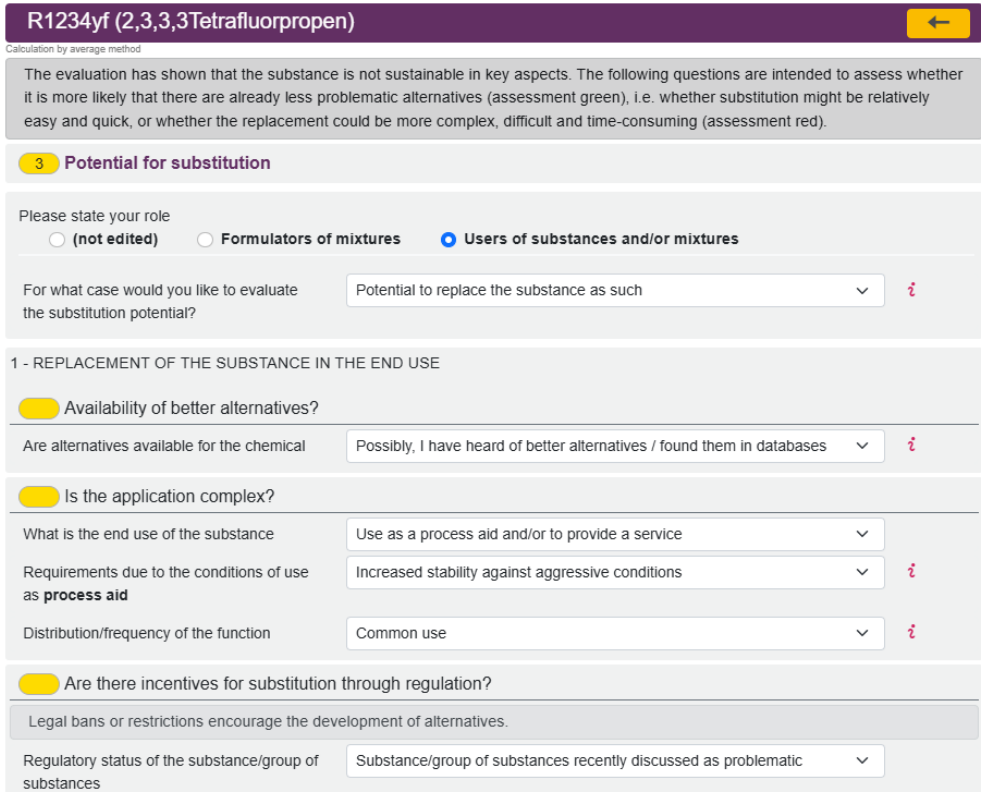
R1234yf



Because of including the PMT/vPvM property of R1234yf's breakdown product TFA, also R1234yf itself is evaluated as a PMT in this example. For the risk indication, PMTs are considered as of very high concern for the environment and consumers. As a consequence, and according to EU risk assessment principles, any such exposure is evaluated as of concern (red). Consumers may be exposed via the environment, e.g. via drinking water. The environment is directly exposed and concentrations of persistent chemicals continuously build up. For workers, only exposures from the workplace are considered and hence, the PMT/vPvM properties do not play a role in the derivation of the risk indication.
The propane is not evaluated as hazardous to either human health or the environment, and hence the indication of risk is green for workers and the environment. It is "not relevant" for consumers, because no immediate contact occurs and – as propane is not persistent – the exposure of consumers is considered as "not relevant".

The life cycle impacts of R1234yf is evaluated as yellow mainly due to the high resource consumption and ozone depletion due to emissions of other, ozone depleting substances, during the production.

3.11 Substitution potential



The substitution potential of propane is not evaluated as no red result is displayed in the summary. Propane can be used as a replacement for R1234yf and therefore, the assessment of the substitution potential ends with selecting the option that alternatives are available.

4 Sustainability comparison

Sustainability comparison for substances

Material	Propane	R1234yf (2,3,3,3Tetrafluorpropen)
Problem substance lists	1 Rank 1	1 Rank 1
Phys. chem. properties	5 Rank 2	3 Rank 1
Human toxicity	1 Rank 1	1 Rank 1
CMR	1 Rank 1	1 Rank 1
Skin/Eye	1 Rank 1	1 Rank 1
Endocrine	1 Rank 1	1 Rank 1
Other damage	1 Rank 1	1 Rank 1
Environmental toxicity	1 Rank 1	5 Rank 2
Aquatic Tox.	1 Rank 1	3 Rank 2
PBT/vPvB + Remote	1 Rank 1	1 Rank 1
PMT/vPvM	1 Rank 1	5 Rank 2
Endocrine	1 Rank 1	1 Rank 1
Exposure potential in workplaces	1 Rank 1	1 Rank 1
Exposure potential consumers	-2	-2
Exposure potential environment	1 Rank 1	1 Rank 1
Climate and ozone	1 Rank 1	3 Rank 2
Global warming potential	1 Rank 1	1 Rank 1
CO2 emissions	1 Rank 1	5 Rank 2
Ozone depletion	1 Rank 1	3 Rank 2
Resource consumption	3 Rank 1	5 Rank 2
Energy	1 Rank 1	5 Rank 2
Water	1 Rank 1	5 Rank 2
Raw materials	3 Rank 1	3 Rank 1
Circularity	1 Rank 1	1 Rank 1
Recovery	1 Rank 1	1 Rank 1
Pollution	1 Rank 1	1 Rank 1
Supplier's responsibility	3 Rank 1	3 Rank 1
Worker	1 Rank 1	1 Rank 1
Environment	3 Rank 1	3 Rank 1
Social environment	3 Rank 1	3 Rank 1

When comparing the two substances, it is obvious that R1234yf is rated red more often than propane. In addition, a central criterion, environmental toxicity, is rated red, which has a particularly high weight. It must be noted, that this is due to including TFA, a degradation product of R1234yf in the assessment. As no possibilities exist to include information about classification proposals, it was decided not to include this in the assessment, but to wait for the official decision.

Among the criteria relating to chemical safety, propane only has a red rating for PC properties. This suggests that propane is a good alternative to R1234yf from a sustainability perspective. ChemSelect cannot assess the technical feasibility.

5 Additional assessment aspects

In this example, the fact that the refrigerant R1234yf breaks down to trifluoro acetic acid (TFA) was considered in the assessment by attributing its hazardous properties to the parent compound R1234yf for the environment, while only keeping it in mind for human health due to a lack of respective opportunities to enter uncertainties in classification. In order to remain simple, and as many downstream users of chemicals lack respective information, ChemSelect does not foresee or ask for the assessment of breakdown products but the assessment focuses on the substances as used. However, if information is available on e.g. the ecotoxicity and toxicity of breakdown products can be considered, as shown in the example. It is good to document this explicitly.

The ozone depletion potential (ODP) of R1234yf was also entered into the tool by not only considering the substance as such, but also emissions from the production process. During research on R1234yf's (ODP), the information about emissions of substances that do harm the ozone layer during the production of R1234yf was found by coincidence. As these emissions are most likely related to halogenated compounds (fluorine-containing ones), it can be assumed that not similar emissions would occur for propane.

The assessment of exposure potentials is different for gases than it is for non-gaseous substances as normally, the release of gases mainly happen during one specific life stage and the exposure main exposure pathways are inhalation (humans) and air (environment). This is due to the fact that either the release is intended (at a specific stage) or the release is not intended and hence occurs during the waste stage. As gases are hard to contain, significant release normally does not spread over several lifecycle stages, allowing for an assessment short-cut where only the one relevant lifecycle stage is identified.

6 Conclusions

R1234yf performs better than propane when it comes to PC properties, because it is non-flammable. However, there is a higher environmental toxicity due to its degradation product TFA; and possibly also due to a future classification as reprotoxic, in the human toxicity criterion. This is generally considered to be more relevant for the sustainability assessment than the PC properties, as the latter are predominantly relevant in the workplace and frequently can be controlled with risk management measures.

The exposure potential does not differ for the gases since the application situation is unchanged.

In terms of environmental impact, R1234fy performs worse than propane, although there is only an estimate for CO2 emissions in production based on the comparison lists, but no data from databases. In addition, the formation of ozone-depleting substances during the production of R1234yf was taken into account when assessing ozone depletion. The ODP of the substance itself is "0", i.e. without this consideration it would also be rated green.

Although not present as a separate feature, ChemSelect users can account for the degradation and intermediates of chemicals (in this case, the degradation of R1234yf to trifluoroacetic acid), if they implicitly include the properties of degradation products in the assessment of the parent compound / precursor. In this example, this is central to the overall evaluation.