Sodium laureth sulphate

Sodium laureth sulphate or sodium lauryl ether sulfate (SLES) is an example of anionic surfactant. It belongs to the Alcohol ethoxysulphates (AES) group. AES are a widely used class of anionic surfactants and found in household cleaning and personal care products. The structure of AES could be described by any of the following formulas:

1- $C_nH_{2n}(C_2H_4O)_mSO_4X$, where n=12-18 and m = 0-8 and X = sodium, ammonium or triethanolamine (TEA)
2- $R_1\text{-}CH_2\text{-}CH_2\text{-}O\text{-}(CH_2—CH_2\text{-}O)_n\text{-}SO_3^-Na^+$ where $R_1 = C_{10\text{-}14}$; n = 1-4.

As part of the PBT assessment of sodium laureth sulphate data from structurally analogous substances (other AES) will be used to fulfil some endpoints for the assessed substance (SDA, 1991; HERA, 2003).

An assessment of the PBT status of Sodium laureth sulphate using the algorithm described in the toolbox is explained below step by step.

Step 1: Substance identification

Identifiers on sodium laureth sulphate have been obtained from the most recent reliable sources (www.chemfinder.com) which is listed in step1. The smiles notation for sodium laureth sulphate was obtained form chemspider and chemID plus source. These identifiers are shown in Table1 below.

Identifier of Sodium laureth sulphate	
EINECS or ELINCS number	239-925-1
CAS name and CAS number	9004-82-4
Name(s) in the IUPAC nomenclature or other international chemical name(s)	Sodium dodecylpoly(oxyethylene) sulphate
Other names (usual name, trade name, abbreviation)	Sodium laureth sulfate; Dodecyl alcohol, monoether with polyethylene glycol, hydrogen sulfate sodium salt; Sodium polyethoxyethyl dodecylsulfate; Polyethylene glycol, mono(hydrogen sulfate), dodecyl ether, sodium salt; Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(dodecyloxy)-, sodium salt; Poly(oxyethylene) lauryl ether sulfate

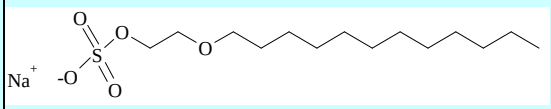
	sodium salt; Sodium polyoxyethylene monoalkyl ether sulfate;
Information related to molecular and structural formula of Sodium laureth sulphate	
Molecular Formula	$C_{14}H_{29}NaO_5S$
Structural formula	
Smiles Notation	[Na+].[O-]S(=O)(=O)OCCOCCCCCCCCCCCC

Table1: Sodium laureth sulphate identification parameters.

Step 2: Data needed for the assessment

These are divided into the followings:

- Physical-chemical properties (water solubility, Partition coefficient n-octanol/water, Soil Adsorption Coefficient (Koc/Kd), and Henry's Law Constant)
- Degradation, (biodegradation, half lives)
- Accumulation (BCF)
- Environmental Partitioning (MacKay)
- Ecotoxicity data of the substance (LC_{50}, NOEC)

Step 3: Collecting the available information and identifying the data gap

1- Information on the physical-chemical properties for Sodium laureth sulphate

The following table provides a summary of the

1. Chemical and physical properties required for the assessment as explained in the algorithm.
2. The available chemical and physical properties of Sodium laureth sulphate along with the source for these data. Unfortunately no IUCLID, MSDS data found for Sodium laureth sulphate. However, a Human Environmental Risk Assessment (HERA) report on Alcohol Ethoxysulphatest group was found in

the www.heraproject.com. Some data related to SLES were reported in this report since it belongs to ASE category.

3. The data gap which is highlighted as red in the table.

Required Property	Value	Source
Water solubility	Very soluble 187mg/l (estimate)	HSDB and HERA (2003)
Partition coefficient n-octanol/water	No measured logK_{ow} is available. Log K_{ow} = 1.62 (calculated)	HERA (2003)
Soil Adsorption Coefficient (Koc/Kd)	No measured log Koc value is available for Sodium laureth sulphate.	
Henry's Law Constant	No experimentally determined Henry's law constant information is available.	

Table2: Physical chemical data available for Sodium laureth sulphate.

2- Accumulation data of Sodium laureth sulphate

No accumulation data were provided for Sodium laureth sulphate. However, an environmental assessment report has been published by the Danish EPA (Masden et al, 2001), which contains studies carried out to determine the BCF values for analogue alkyl ether sulfates. Based on these studies, the report concludes that AES is not considered to bioconcentrate in aquatic organisms.

3- Degradation data of Sodium laureth sulphate

The following table provides a summary of the

1. Degradation properties required for the assessment as explained in the algorithm.
2. The available degradation data of Sodium laureth sulphate along with the source for these data. As explained in the algorithm, the data should be reliable.
3. The data gap which is highlighted as red in the table.

Required Property	Value	Source
Biodegradation	On the basis of the available data, Sodium laureth sulphate is considered to be readily biodegradable under aerobic and anaerobic conditions and easily degradable both primarily and ultimately (study conducted according to OECD TG 301C guideline)	HERA (2003)
Half lives-$t_{1/2}$		
1-Hydrolysis as a function of pH 2-Photolysis (Atmospheric OH Rate Constant)	No experimental aquatic degradation data are available for Sodium laureth sulphate. No experimental data are available for Sodium laureth sulphate only calculated one Rate Cons = 1.67 *10-11	

Table3: Degradation data available for Sodium laureth sulphate.

4- Environmental Partitioning (MacKay)

No data was available.

5- Aquatic toxicity information of Sodium laureth sulphate

Aquatic toxicity data for structurally similar compounds have been identified in several sources (HERA risk assessment, Masden et al, 2001). The data are summarised below in Table 4.

Required Property	Value	Source
Fish Acute toxicity to fish (96hrs LC_{50}) mg/l	The 24-96 h LC50 values for seven different fish species range between 0.39 mg/L to 450 mg/L. The toxicity of AES with chain length $<C_{16}$ decreases with increasing numbers of EO groups and peaks at chain lengths of C_{16}.	HERA, Masden2001
Long term toxicity to fish (28days NOEC) mg/l		
Daphnia Acute toxicity to Daphnia (48hrs EC_{50}) mg/l	For Daphnia magna, the acute EC50 values range between 1 and 50 mg/L were reported for AES.	
Long term toxicity to Daphnia (21days NOEC) mg/l		
Algae Acute toxicity to algae (72hrs EC_{50}) mg/l	For algae, typical EC50 values range from 4 to 65 mg/L. For AES with chain lengths in the same range as Sodium laureth sulphate, the 21 day EC50 is 20 mg/L for C_{12-14} AE_nS, the 72 h EC50 is 32 mg/L for C_{12-14} AES and the 48 h EC50 is 65 mg/L for C_{10-15} AE_3S.	HERA, Masden2001

Table4: Aquatic toxicity data available for Sodium laureth sulphate.

Step 4: Filling the data gap by using QSAR

In this step the above endpoints (both the available and not) will be predicted using QSARs tools and software listed in step 4 of the algorithm (EPIWIN, Danish(Q)SAR data base and PBT profiler). The reason for doing this is to compare the QSAR results with the experimental one to identify the accuracy of the QSAR.

1- Results obtained by using EPIWIN

Table 5 provides the predicted values for the above endpoints using EPIWIN software along with the name of the programme used. The output obtained by EPIWIN for each end point is given. Also included are explanation which in the toolbox would be obtained by clicking on a link to view. An interesting point found in this step. As explained in the algorithm that one way to enter the chemical into EPIWIN program is by typing its CAS registry number. An automatic look-up function based on the CAS Registry number is then automatically retrieving the chemical's SMILES notation using a pre-existing database containing over 100,000 records (SMILESCAS

database). However, in our case when entering the CAS NO of 9004-82-4 corresponding to Sodium laureth sulphate, a different SMILES notation appeared and therefore not the right chemical (click here to view an example). Accordingly, to get the correct estimate for Sodium laureth sulphate using EPIWIN the chemical was entered into the program by typing its SMILES notation; [Na+].[O-]S(=O)(=O)OCCOCCCCCCCCCCCC.

Required Property	**EPI QSAR Programme**	**Predicted Value**
Water solubility	WSKOW (result output)	486.5 mg/l at 25 C
Partition coefficient n-octanol/water	KOWWIN	Log K_{ow} = 1.42
Bioconcentration Factor (BCF)	BCFWIN	LogBCF = 1.85 (BCF =70.79)
Soil Adsorption Coefficient (Koc/Kd)	(PCKOCWIN)	K_{oc} = 3489
Henry's Law Constant	HENRYWIN	2.86 *10^{-9} atm-m^3/mole
Half lives-$t_{1/2}$		
1-Hydrolysis as a function of pH	HYDROWIN	Can not be estimated
2-Photolysis (Atmospheric OH Rate Constant)	AOPWIN	Atmospheric Oxidation Rate Constant is approximately around 31.46 E-12 cm^3/molecule-sec Half-Life = 4hrs
(Atmosph. Oxidation, Ozone)	AOPWIN	Can not be estimated
Biodegradability		
BIOWIN1	BIOWIN	0.35 (Does not Biodegrade fast)
BIOWIN2	BIOWIN	0.36 (Does not biodegrade fast)
BIOWIN3 (Ultimate biodegradation)	BIOWIN	2.75 (weeks)
BIOWIN4 (Primary Biodegradation)	BIOWIN	3.63 (Days-weeks)
BIOWIN5	BIOWIN	0.37 (Not readily Degradable)
BIOWIN6	BIOWIN	0.17 (Not readily Degradable)
BIOWIN7	BIOWIN	0.52 (biodegrades fast)
Ready Biodegradability Prediction:	BIOWIN	NO
Environmental Partitioning		

(MacKay)	EPI V3.2 (Results output)	Level III Fugacity Model: Mass Amount (percent) / Half-Life (hr) / Emissions (kg/hr) Air 1 / 8.6 / 1000 Water 36 / 360 / 1000 Soil 64 / 720 / 1000 Sediment 0 / $3.24*10^3$ / 0
Fish Acute toxicity to fish (96hrs LC50) mol/l Long term toxicity (28days NOEC) mol/l	ECOSAR	Can not be estimated
Daphnia Acute toxicity to Daphnia (48hrs EC_{50}) mol/l Long term toxicity (21days NOEC) mol/l	ECOSAR	Can not be estimated
Algae Acute toxicity to Algae (72hrs EC_{50}) mol/l	ECOSAR	Can not be estimated

Table5: EPIWIN predictions of the required endpoints

2- Results obtained from Danish(Q)SAR database

Unfortunately, no data was found for Sodium laureth sulphate using the Danish(Q)SAR database. The search revealed no matches. However other QSAR databases could be used such as chemspider or PBT profiler. Chemspider provides an online access to structure based predictions of systematic identifiers and physicochemical based predictions. You only need to type the name of your chemical, click on search and the predictions result will appear. The problem in using this source is that information about the QSARs models used for the prediction is not available. On the other hand, PBT Profiler is a no-cost computer based tool to screen chemicals lacking experimental data in order to help identify if they are potentially may persist, bioaccumulate, and be toxic to aquatic life, i.e., PBT chemicals. The good thing with PBT profiler, is that it provides a straight-forward estimate of persistence, bioaccumulation, and aquatic toxicity based on widely accepted criteria along with the explanation of the results. It is important to know that the PBT Profiler is a screening level predictive tool and cannot be used for all chemical substances.

Similarly to EPIWIN program finding, when entering Sodium laureth sulphate into PBT profiler via its CAS NO (9004-82-4), a different structure to Sodium laureth sulphate was found. The PBT profiler report for a chemical with CAN no of 9004-82-4 was for sodium lauryl ether sulfate as shown in figure1. In fact, this was expected

since PBT profiler is linked to the same SMILESCAS database that EPIWIN program make use of.

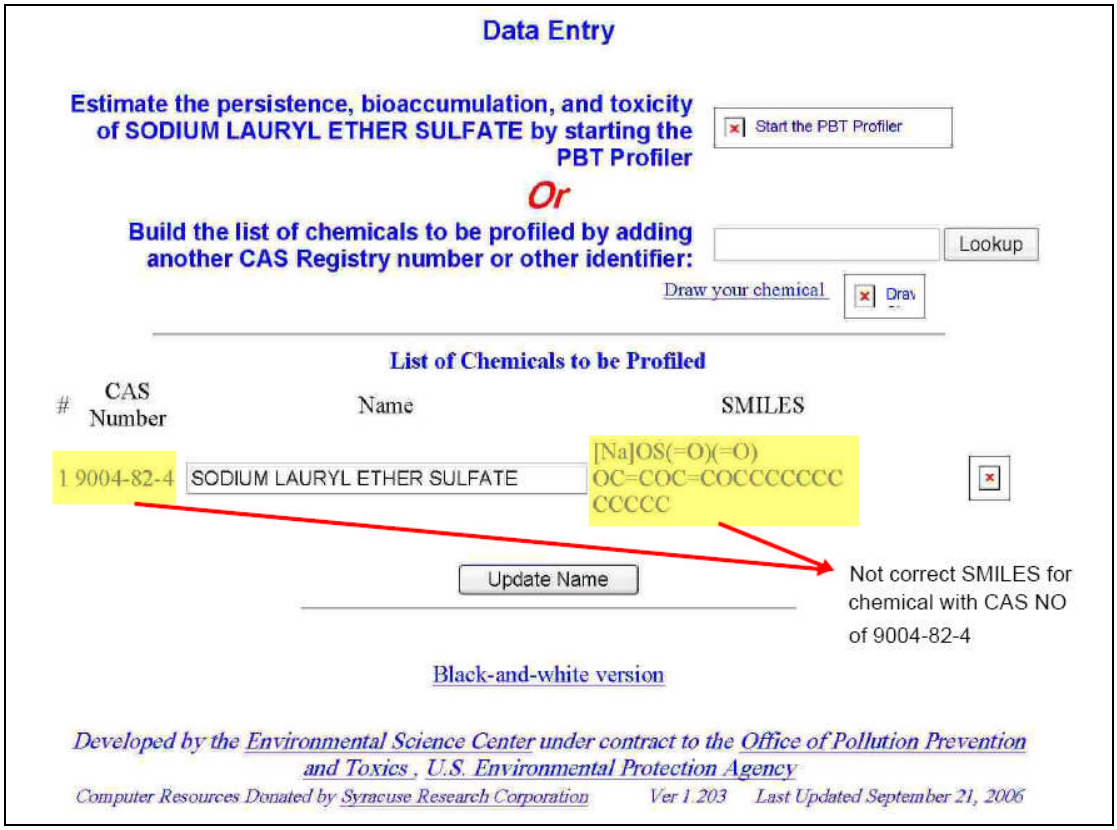


Figure 1: PBT profiler data entry output for a chemical with CAS No of 9004-82-4.

To get the PBT profiler report for Sodium laureth sulphate, the chemical was entered into the tool via its name and SMILES notation. The PBT profiler report for Sodium laureth sulphate with some comments is shown in the Figures below. These outputs contain predictions for environmental Partitioning (MacKay), BCF, fish chronic toxicity (Figure2) along with some physical/chemical properties (Figure3).

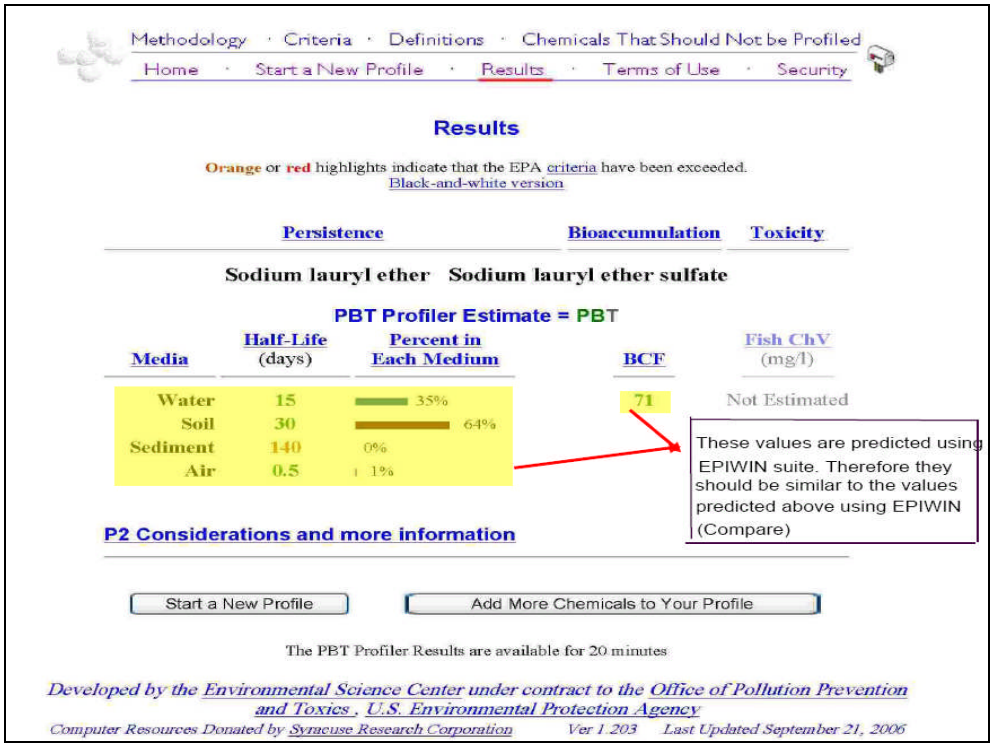


Figure2: PBT profiler report output for Sodium laureth sulphate.

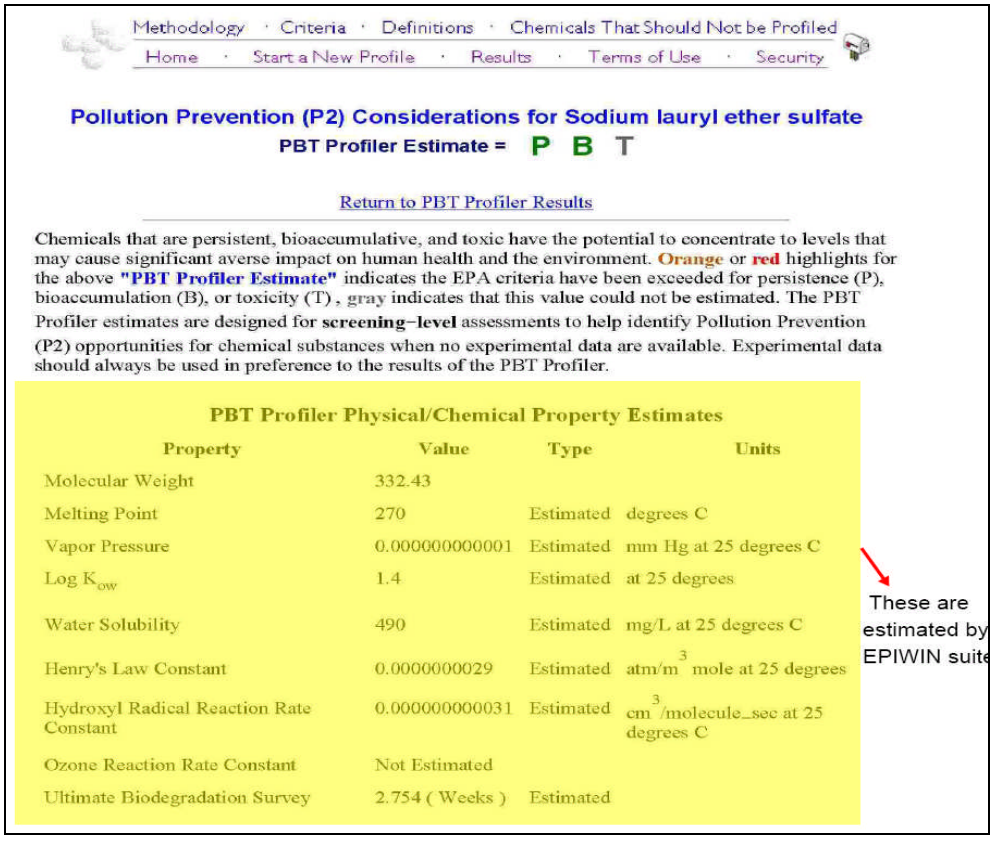


Figure3: PBT profiler report output for Sodium laureth sulphate.

Before proceeding to step 5, it is useful to compare the predicted values obtained from EPIWIN with PBT profiler results. By doing this, the reproducibility of EPIWIN predictions can be tested since the PBT estimates are based on EPIWIN.

As expected, the available QSAR-predictions from the EPIWIN suite are in line with the one obtained from PBT profiler (Log K_{ow}, Henry's Law Constant and Environmental Partitioning (MacKay (III), see Table 6).

Required Property	**Predicted Value using PBT profiler**	**Predicted Value using EPIWIN**
Water solubility	420 mg/l	486 mg/l at 25 °C
Partition coefficient n-octanol/water	log K_{ow} = 1.4	log K_{ow} = 1.4
Bioconcentration Factor (BCF)	BCF = 71	BCF = 71
Henry's Law Constant	0.0000000029 atm-m^3/mole	2.86 *10^{-9} atm-m^3/mole
Photolysis (Atmospheric OH Rate Constant)	Rate constant =0.000000000031	Rate Constant = 31. 46 E-12 cm3/molecule-sec
Ultimate biodegradation	2.75 (weeks)	2.75 (weeks-months)
Environmental Partitioning (MacKay, (III))	Mass Amount (percent) / Half-Life (days) Air 1 / 0.5 Water 35 / 15 Soil 64 / 30 Sediment 0 / 140	Level III Fugacity Model: Mass Amount (percent) / Half-Life (hr) Air 1 / 8.6 Water 35 / 360 Soil 64 / 720 Sediment 0 / 3.24*10^3

Table6: Comparison between the results obtained from EPIWIN with PBT profiler.

Step 5: Assess your substance to identify whether it is PBT or vPvB

The assessment of persistence is based on the degradation data (biotic and chemical) and on the half life data.

Based on available data for structurally-similar compounds AES, Sodium laureth sulphate is expected to biodegrade rapidly in the environment. This is in contrast to the predictable results by BIOWIN (see table 5). However the assessment of biodegradability will be based on the experimental data since it is available.

Moreover, the predicted rate constant and estimated half-life for the reaction of hydroxyl radicals with Sodium laureth sulphate in the atmosphere indicated that when Sodium laureth sulphate is released to the atmosphere is likely to be degraded (not persistence) by this fate process. As a result, these data suggest that Sodium laureth sulphate is unlikely to be persistent. In addition, both PBT Profiler and EPIWIN v3.2 estimate for Level III Fugacity Model have estimated that Sodium laureth sulphate is expected to be found predominantly in soil. However, its half-life in soil is 30 days, does not exceed the EU criteria of >120 days. Therefore, Sodium laureth sulphate is estimated to be not persistent in the environment.

As a conclusion, based on the available data (measures and predicted) degradation and half life, Sodium laureth sulphate is not considered to meet the screening criteria for persistence.

Is your substance bioaccumlative?

No measured BCF data is available. The potential for bioaccumulation was therefore assessed on the basis of a calculated BCF.

Both PBT profiler and BCFWIN v2.17 predict BCF of 71 (<2000, not accumulative) based on $\log K_{OW}$ of 1.4.

Based on this value Sodium laureth sulphate is not considered to meet the screening criteria for bioaccumulation.

Is your substance toxic to the environment organisms?

Aquatic toxicity data for structurally similar compounds have been identified in several sources (HERA risk assessment, Masden et al, 2001). The acute toxicity values L(E)C50 for fish and Daphnia reported for AES ranged between 0.39 mg/L to 450 mg/L and 1 and 50 mg/L respectively. These values are clearly above 0.1 mg/l and therefore Sodium laureth sulphate is not considered to meet the screening criteria for aquatic toxicity. In addition, Ying claimed that most surfactants are not acutely toxic to organisms at environmental concentrations and their aquatic chronic toxicity occurs usually at concentrations above than 0.1mg/l apart of alkylphenols surfactants.

In conclusion, based on the available aquatic toxicity data, Sodium laureth sulphate is not considered fulfilling the T screening criterion related to aquatic toxicity.

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Is your chemical classified as potential PBT?

Based on the available data, the substance has been shown to have a half-life of 30 days <180 days in soil and biodegrades fast. Therefore the substance does not fulfil the P-criterion. The estimated BCF for the substance in fish is 71 (<2000) and therefore the substance does not fulfil the B-criterion. The reported aquatic toxicity data for Sodium laureth sulphate suggests that the substance does not fulfil the T-criterion related to aquatic toxicity.

Therefore on the basis of the predictions and measured data the substance should not be considered as potential PBT.

What is the preferred environmental compartment of your chemical? (Environmental Distribution)

Adsorption:

The substance has a high K_{oc} value of 3498 indicating that the substance is likely to adsorb onto soil. This is also in agreement with the Mackay level III predictions, which shows that that soil is the preferred environmental compartment (64%). Therefore the persistence of Sodium laureth sulphate in soil is probably more significant than the persistence in water.

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