TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

Substance name: Resin acids and Rosin acids, sodium salts

EC number: 263-144-5

CAS number: 61790-51-0

Molecular formula: not applicable (substance is a UVCB)

Structural formula: not applicable (substance is a UVCB)

Summary of the evaluation

Resin acids and Rosin acids, sodium salts is considered to be a UVCB substance. Based on screening data it is not fulfilling the PBT/vPvB criteria.

Resin acids and Rosin acids, sodium salts is considered as a substance with a potential PBT/vPvB constituent (based on screening data). This conclusion need not apply in case it can be shown, that the concentration of this impurity is < 0.1% w/w.

Resin acids and Rosin acids, sodium salts may contain sesquiterpenes (which itself is a mixture) as a constituent, which may fulfil the PBT criteria based on QSAR-estimates of the most common sesquiterpene β –caryophyllane.

A test on ready biodegradation is available with Resin acids and Rosin acids, sodium salts showing ready biodegradation of the test substance. The P-screening criterion is therefore not fulfilled. Regarding the B-criterion, only QSAR values are available both with respect to the log Kow and the BCF. BCFwin and Kowwin predict different values for Log Kow; 6.46 and 2.65, respectively. The calculated BCF is 56, when using a log Kow of 6.46 for calculation. The B-screening criterion is therefore not fulfilled. Based on acute aquatic toxicity results with L/EC_{50} above 2 mg/L the screening T-criterion is not fulfilled.

Data on individual constituents are not available. Based on QSAR there is no clear picture regarding persistence, bioaccumulation and toxicity because the constituents have pKa values around environmentally relevant pH values. However, no further testing is considered necessary as Resin acids and Rosin acids, sodium salts is readily biodegradable.

JUSTIFICATION

1. Identification of the Substance and physical and chemical properties

Table 1.1: Identification of resin acids and rosin acids, sodium salts

Name	Resin acids and Rosin acids, sodium salts
EC Number	263-144-5
CAS Number	61790-51-0
IUPAC Name	-
Molecular Formula	not applicable
Structural Formula	not applicable
Molecular Weight	not applicable
Synonyms	Sodium salt of rosin Sodium soap of disproportionated rosin

1.1 Purity/Impurities/Additives

Resin acids and Rosin acids, sodium salts (CAS no 61790-51-0) is a UVCB (Substance of Unknown, Variable Composition, or of Biological Origin), which consists mainly of the salt of a complex mixture derived from wood. The mixture is composed primarily of resin acids and modified resin acids such as dimers and decarboxylated resin acids. The composition of the substances varies among other factors due to the raw material and the production process.

The major constituents of the sodium salts are shown as acids in the following table. The relative content of the acid salts depends on the source and further processing (disproportioning) (according to HARPA's Environmental Test Program, 1998). The values given are examples.

Table 1.2 Composition of Resin acids and Rosin acids, sodium salts according to HARPA's Environmental Test Program, 1998.

Trivial name	CAS-no.	Rosin Content (%)	Disproportionated rosin Content (%)
Abietic acid	514-10-3	44.5	0
Dehydroabietic acid	1740-19-8	2.9	54.0
Palustric acid	1945-53-5	17.9	0
Isopimaric acid	5835-26-7	3.4	3.4
Neoabietic acid	471-77-2	15.8	0
Pimaric acid	127-27-5	7.3	7.3
Levopimaric acid	79-54-9	0.7	0
Sandaracopimaric acid	471-74-9	1.5	1.5
Sesquiterpenes	mixture	4.4	0
Unidentified	-	1.6	10.0
Dihydroabietic acid		0	23.8
Total		100	100

The cations of sodium, potassium, calcium and magnesium salts, listed in table 1.3, should be regarded as a group. It should also include all combinations with these cations as well as disproportionated, dehydrogenated rosin.

Table 1.3 CAS numbers of salts of tall oil rosin and rosin to be considered as corresponding substances to resin acids and rosin acids.

CASnumber	**EINECS**	**Name**
61790-51-0	263-144-4	Resin acids and Rosin acids, sodium salts
61790-50-9	263-142-4	Resin acids and Rosin acids, potassium salt
9007-13-0	232-694-8	Resin acids, and rosin acids, calcium salt
68440-56-2	270-461-2	Resin acids and Rosin acids, magnesium salt
84776-85-2	284-011-8	Resin acids and Rosin acids,, tall-oil, potassium salt
85409-26-3	287-093-3	Resin acids and Rosin acids, tall-oil, sodium salt
68512-67-4	270-987-2	Resin acids and Rosin acids, potassium salt

1.2 Physico-Chemical properties

Physico-chemical properties are available in IUCLID (European Commission, 2000) for resin acids and rosin acids, sodium salts.

Table 1.4 Physico-chemical properties resin acids and rosin acids, sodium salts

REACH ref Annex, §	Property	Value	Source
VII, 7.1	Physical state	Solid or liquid	IUCLID (2000)
VII, 7.2	Melting point	67 °C	Les Derives Resiniques et Terpeniques Dax
VII, 7.3	Boiling point	> 100 °C	Eka Chemicals Ltd Weston-super-Mare
VII, 7.4	Relative density	Density: 1.1 kg/m^3 at 20 °C	Eka Chemicals Ltd Weston-super-Mare
VII, 7.5	Vapour pressure	< 25 hPa at 20 °C	Eka Chemicals Ltd Weston-super-Mare
VII, 7.7	Water solubility	No data available "infinitely miscible with water", pH 9.5 and 25 °C	Eka Chemicals Ltd Weston-super-Mare
VII, 7.8	Partition coefficient n-octanol/water (log value)	> 3 (OECD 117)*	Les Derives Resiniques et Terpeniques Dax
VII, 7.16	Dissociation constant	No data available	-

No experimental data on the individual constituents of the mixture (as presented in Table 1.2) are available and therefore water solubility and log Kow have been estimated with QSAR.

Table 1.5 Water solubility and logKow of the constituents of resin acids and rosin acids, sodium salts

QSAR	Water sol.	Water sol.	log Kow
	(WATERNT, v1.0)	(WSKOWWIN v1.41)	(KOWWIN, v1.67)
Abietic acid*:	0.28 mg/l	0.09 mg/l	6.46
Dehydroabietic acid:	0.13 mg/l	0.08 mg/l	6.52
Palustric acid:	0.44 mg/l	0.02 mg/l	7.27
Isopimaric acid:	0.19 mg/l	0.09 mg/l	6.44
Neoabietic acid:	0.44 mg/l	0.07 mg/l	6.59
Pimaric acid:	0.19 mg/l	0.09 mg/l	6.45
Levopimaric aicd:*	0.28 mg/l	0.09 mg/l	6.46
Sandaracopimaric acid:	0.19 mg/l	0.09 mg/l	6.45

In QSAR there is an experimental value available for water solubility of abietic acid, which is 48.4 mg/L. This is considerably higher than the calculated value and may be a result of the pH dependency of the water solubility of abietic acid. Abietic acid and the other constituents have pKa values at environmentally relevant pH values; however, no experimental data are available.

Several pKa values have been found in the scientific literature:

- Luong et al. 1999 quotes that "At pH below their pKa (< 5.7-6.4) the resin acids were virtually unionized and insoluble"
- In Kamaya et al. 2005 for dehydroabietic acid pKa values between 5.7 and 7.25 and 6.4-7.15 for abietic acid are given

- In Nyren and Back 1958 pKa values for abietic and dehydroabietic acid are 6.4 and 5.7, respectively, were reported
- Cited by Hall and Liver 1996 were pKa values for abietic and dehydroabietic acid of 7.15 and 7.25, respectively

PKa values for the constituents of resin acids and rosin acids, sodium salts were also predicted using the SPARC software (Version 1.4, released January 2008). Values of 4.7 to 4.8 were predicted and these are considered consistent with expectations for a carboxylic acid functional group. The predicted values are considered reliable as the method has been validated with a number of carboxylic acids. Predicted pKa values for 9 carboxylic acids (pKa 4.0-4.8) have been compared with measured pKa values for these acids obtained from the literature (pKa 4.2-5.0).

2 MANUFACTURE AND USES

Seven companies have notified the substance under Regulation 93/793 EEC according to IUCLID (European Commission, 2000). The substance is used in quantities between 10,000 – 50,000 tons per year (European Commission, 2000).

The substance is a UVCB. Resin acids and rosin acids, sodium salts are produced by saponification of gum or tall oil rosin which itself is derived from the living tree or as a by-product from the Kraft process for wood pulping. The resin acids are diterpene carboxylic acids based on an alkyl-substituted perhydrophenanthrene ring structure and the fatty acids are predominantly 18-carbon, straight-chain mono- or diunsaturated fatty acids.

3 CLASSIFICATION AND LABELLING

The substance is not classified under Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

No data available.

4.1.2 Biotic degradation

According to IUCLID 35 % biodegradation after 28 days is indicated in a closed bottle test according to OECD 301D (1981). A newer OECD 301D biodegradation study from 1991 with gum rosin (CAS no. 8050-09-7) resulted in a biodegradation of 71 % after 28 days. The study is valid as the reference compound sodium acetate was degraded by 69 % of its theoretical oxygen demand after 14 days. Oxygen concentration was > 0.5 mg/L in all bottles during the test period. This supports a classification of "readily biodegradable" on the CAS no. 8050-09-7. The test report on gum rosin is assessed to be representative for the CAS no. 61790-51-0 (resin acids and rosin acids, sodium salt). However, the study was performed for the whole mixture and does not give information whether (smaller) fractions of persistent substances are present in the mixture.

To assess biodegradation of the constituents QSAR predictions have been conducted.

Table 4.1 Persistency of possible constituents in CAS no 61790-51-0.

	BIOWIN 2 v4.10	BIOWIN 3 v4.10	BIOWIN 6 v4.10
Abietic acid	0.0165	2.4711	0.044
Dehydroabietic acid	0.0518	2.326	0.0561
Palustric acid	0.0165	2.4711	0.0606
Isopimaric acid	0.003	2.259	0.0907
Neoabietic acid	0.0165	2.4711	0.0589
Pimaric acid	0.003	2.259	0.0907
Levopimaric acid	0.0165	2.4711	0.044
Sandaracopimaric acid	0.003	2.259	0.0907

Sesquiterpenes

Resin acids and Rosin acids, sodium salts contain sesquiterpenes, which is a mixture itself. There are over 3000 sesquiterpene and sesquiterpenealcohol structures that have been isolated and identified in nature. The most common sesquiterpene is β – caryophyllane.

Table 4.2 BIOWIN

	BIOWIN 2 v4.02	**BIOWIN 3 v4.02**	**BIOWIN 6 v4.02**
β -caryophyllane	0.17	2.54	0.13

It is mentioned in fact sheet no. 84 that the applicability of BIOWIN for monoterpenes and β-caryophyllane is questionable, because the program does not calculate any fragment corrections for specific substructure entities and uses instead a molecular weight correction factor. The quaternary carbons are identified as "carbon with 4 single bonds and no hydrogens" without distinguishing the cyclic structure they are connected with.

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

According to the test results from a closed bottle test (OECD 301D) on resin acids and rosin acids, sodium salts was found not to be readily biodegradable. However, results from another closed bottle test (OECD 301D) on the CAS n. 8050-09-7 (gum rosin) from 1999 are considered more reliable and showed that the test substance is readily biodegradable (71 % after 28 days). The test report on gum rosin is assessed to be representative for the CAS no 61790-51-0 (resin acids and rosin acids, sodium salts).

Biodegradation has been predicted by QSAR for the respective constituents of the mixture. According to the predictions, the constituents behave very similarly and can be considered a borderline case between being readily and not readily biodegradable. According to the TGD a substance can be considered to be not readily biodegradable when the non-linear model prediction is <0.5 or the MITI non-linear model prediction is < 0.5 and the ultimate biodegradation timeframe prediction is < 2.2. Biowin 3 predictions show values between 2.3-2.5. This would mean that all constituents can be considered as being readily biodegradable when looking at the figures in table 4.1. However, according to REACH RIP 3.3 (Guidance on information requirements) a substance can be regarded as borderline case with respect to the ready biodegradation if the estimate of the ultimate degradation time (Biowin 3) gives a result in the range 2.2 to 2.7.

[1] For example, half life from field studies or monitoring data

In conclusion, a valid biodegradation test with the mixture is available and showed ready biodegradation. The known constituents comprise of more than 80 % of the mixture and therefore the mixture can be considered readily biodegradable. However, minor fractions of persistent substances might be present in the mixture.

According to the PBT summary fact sheet no. 84 an overall conclusion for the sesquiterpene β-caryophyllane is drawn that the substance, in the absence of experimental data, has to be considered potentially persistent.

4.2 Environmental distribution

No data available.

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data

According to IUCLID the log Kow of resin acids and rosin acids, sodium salts is > 3 (OECD 117). The QSAR estimation gives a BCF value of 56 (BCFwin v2.17), when calculating with a log Kow of 6.46 (estimated with BCFwin v2.17). Log Kowwin predicts a log Kow of 2.65.

The B-criterion of the constituents has been assessed using two different QSAR-programs.

Table 4.2 Log BCF values of constituents of CAS no 61790-51-0

	BCF WIN v2.17 Log BCF	Bintein* Log BCF
Abietic acid	1.75	4.16
Dehydroabietic acid	1.75	-
Palustric acid	1.0	3.59
Isopimaric acid	1.75	4.17
Neoabietic acid	1.75	4.1
Pimaric acid	1.75	4.17
Levopimaric acid	1.75	4.16
Sandaracopimaric acid	1.75	4.17

* Bintein's model included in "OECD (Q)SAR Application Toolbox, Beta version v 0.6. September 2007."

Bintein's model (Bintein et al. 1993) gives log BCF values > 4 for all constituents apart from palustric acid (3.59), while BCFwin gives results < 2. The reason for this difference is most likely that the constituents are ionisable substances and that the pKa values might be around environmentally relevant pH values. Bintein's model is only based on non-ionic substances (Pavan et al. 2006), while BCFwin gives results for ionic substances.

Sesquiterpenes

	Water solubility (mg/L at 25 ºC)	LogKow	Log BCF
β -caryophyllane	0.05 (WSKOW v1.41)	6.3 (KOWWIN v1.67)	4.15 (BCFWIN v2.15 using logKow of 6.3)

4.3.2 Measured bioaccumulation data

Experimentally derived BCF values are not available for resin acids and rosin acids, sodium salts or the constituents.

In the open literature Niimi and Lee (1992) reported experimental BCF values for abietic, dehydroabietic, neoabietic, palustric, pimaric, isopimaric and sandaracopimaric acid. Rainbow trout were exposed to waterborne acids for 20 days to estimate BCF values, followed by a 10 day acid-free period to estimate the elimination rate. The highest BCF found in the study was 220 for neoabietic acid after 10 days. This value declined to 129 at day 20. However, the study has some deficiencies. Fish were exposed to several substances simultaneously and the

exposure period was only 20 days. Given the fact that the pH in the study was around 8 (8.0-8.3) and that these acids might have pKa values around or below 7, it can be assumed that the undissociated acids have not been tested but that the measured BCF values refer to their respective ionic forms.

4.3.3 Other supporting information[2]

No data available.

4.3.4 Summary and discussion of bioaccumulation

Only QSAR values are available both with respect to the log Kow of 6.46 / 2.65 (BCFwin / Kowwin) and the BCF. The estimated BCF of 56 (BCFwin) is based on the ionic form and has to be interpreted carefully.

Experimental data on bioaccumulation are not available for resin acids and rosin acids, sodium salts or the constituents. The screening B-criterion based on a measured log Kow of resin acids and rosin acids, sodium salts and based on the predicted BCF value is not fulfilled. The screening B-criterion based on calculated BCF values for the constituents might be fulfilled dependant on the model used. According to BCFwin the screening B-criterion is not fulfilled, using Bintein's model it is fulfilled. The screening B-criterion for β -caryophyllane is fulfilled.

Theoretically, testing could hence be necessary to determine the actual bioaccumulation potential for the mixture/the constituents. However, testing of the substance as a whole might not be appropriate for this assessment due to variations in the composition of the mixture and the probably large concentration range of the anticipated constituents and impurities.

In conclusion, as resin acids and rosin acids, sodium salts do not fulfil the P-screening criterion further testing on the B-criterion is not considered necessary.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

[2] For example, measured concentrations in biota

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

6.1.1 Toxicity test results

Acute aquatic ecotoxicity studies with resin acids and rosin acids, sodium salts are available with fish, daphnids and algae (see 6.1.1.1, 6.1.1.2 and 6.1.1.3).

The toxicity of the constituents, including β –caryophyllane, has been evaluated with QSAR as no data on ecotoxicity of the constituents are available.

Table 6.1 QSAR values for EC50/LC50 in mg/L for fish, *daphnia magna* and algae.

	OECD Toolbox / Ecosar v0.99h	OECD Toolbox / Ecosar v0.99h	OECD Toolbox / Ecosar v0.99h
	Fish*	Daphnia magna*	Algae*
Abietic acid	0.44 / 0.144	0.01 / 0.21	9.8 / 0.17
Dehydroabietic acid	- / 0.126	- / 0.184	- / 0.149
Palustric acid	0.44 / 0.025	0.01 / 0.038	27.6 / 0.038
Isopimaric acid	0.53 / 0.147	0.01 / 0.214	9.86 / 0.173
Neoabietic acid	0.36 / 0.109	0.01 / 0.160	8.93 / 0.130
Pimaric acid	0.53 / 0.147	0.01 / 0.214	9.86 / 0.173
Levopimaric acid	0.44 / 0.144	0.01 / 0.210	9.79 / 0.170
Sandaracopimaric acid	0.53 / 0.147	0.01 / 0.214	9.86 / 0.173

* E/LC_{50} values in mg/L

Sesquiterpenes

C15H24–terpenes (sesquiterpenes)	
β -caryophyllane	ECOSAR v0.99 : 96 h LC50 = 0.014 mg/L (fish) 48 h EC50 = 0.020 mg/L (daphnia) 96 h EC50 = 0.012 mg/L (green algae) 30 d EC50 = 0.004 mg/L (fish)

6.1.1.1 Fish

Acute toxicity

According to IUCLID the 96 hours LC_{50} values for Resin acids and Rosin acids, sodium salts to Zebra fish were 5-10 mg/L (OECD 203).

Long-term toxicity

No data available.

Endocrine disruption

Extensive research has been conducted for several decades to elucidate the mechanisms of action of endocrine disrupters from pulp and paper mill effluents. While it is acknowledged that paper and pulp mill effluents exhibit endocrine disrupting potential, little information is available to directly link the reported effects observed in fish exposed to these effluents to individual fractions or specific substances.

Although some mechanisms have been identified, the causal agents are poorly characterised. It is, however, suggested that compounds such as terpenoidbased wood components and flavonoids in Kraft effluents are estrogenic, whereas terpenoids and stilbenes may be responsible for effects on the reproductive system of fish exposed to pulp mill effluents (Belknap et al., 2006). An Environment Canada report (McMaster *et al.*, 2004) suggests that that abietic acid and similar compounds may affect endocrine processes in vivo. It is also suggested that the endocrine disrupting compounds in these effluents are biodegradable and poorly bioaccumulative, thus suggesting attained exposure to cause effects. Little if any information is available to verify that these compounds are causing endocrine disrupting effects in vivo.

6.1.1.2 Aquatic invertebrates

Acute toxicity

According to IUCLID 48 hours EC_{50} values for resin acids and rosin acids, sodium salts to *Daphnia magna* were 76 mg/L (OECD 202).

In the literature (Kamaya et al. 2005) measured 48 hours EC_{50} values for D*aphnia magna* for abietic acid (7.98 mg/L) and dehydroabietic acid (7.48 mg/L) are stated. These are considerably higher than the QSAR-estimates.

The difference in toxicity between data from literature and QSAR may be that toxicity of the substances is pH dependent. In the QSAR models calculations are based on non-dissociated molecules, while in toxicity tests, salts of the acids may be present. A good example for the pH dependence of toxicity of these compounds is dehydroabietic acid. For *Daphnia magna* the 48 h EC_{50} increases from 2.47 mg/L at pH 6.5 to 77 mg/L at pH 10 (Zanella 1983; http://smartech.gatech.edu/bitstream/1853/677/1/3355_005_081982.pdf).

Long-term toxicity

No data available.

6.1.1.3 Algae and aquatic plants

According to IUCLID the 72 hours ErC_{50} values for resin acids and rosin acids, sodium salts to *Selenastrum capricornutum* were 18-20 mg/L (OECD 201).

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

No data available.

6.2 Terrestrial compartment

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence

The screening P criterion is not fulfilled for resin acids and rosin acids, sodium salts based on the test result from a ready biodegradation test. Resin acids and rosin acids, sodium salts was shown to be readily biodegradable. As the test was conducted with the mixture, no information is available whether smaller fractions of persistent substances are present in the mixture. Therefore biodegradation of the constituents was predicted by QSAR. The results were quite similar for all constituents. According to the TGD a substance can be considered to be not readily biodegradable when the non-linear model prediction is <0.5 or the MITI non-linear model prediction is < 0.5 and the ultimate biodegradation timeframe prediction is < 2.2. Biowin 3 predictions show values between 2.3-2.5; however, the screening P-criterion might nevertheless be fulfilled for all constituents. According to REACH RIP 3.3 (Guidance on information requirements) a substance can be regarded as borderline case with respect

to the screening P-criterion if the estimate of the ultimate degradation time (BIOWIN 3) gives a result in the range 2.2 to 2.7.

In conclusion, as the mixture is readily biodegradable based on experimental data and the known constituents comprise of more than 80 % of the mixture, it can be concluded that resin acids and rosin acids, sodium salts is readily biodegradable, therefore not fulfilling the P-criterion.

According to the PBT summary fact sheet no. 84 on Terpenes and Terpenoids, turpentine-oil, 3-carene fraction it is concluded that in the absence of experimental data for the most common sesquiterpene β-caryophyllane, an overall conclusion is drawn that the substance is potentially persistent.

Bioaccumulation

A BCFwin estimation gives a log Kow of resin acids and rosin acids, sodium salts of 6.46. Kowwin predicts a log Kow of 2.65. QSAR estimation, based on BCFwin v2.17, result in a BCF value of 56. Based on this data the screening B-criterion is not fulfilled.

Regarding β-caryophyllane the B-screening criterion, based on QSAR data, is fulfilled.

Toxicity

Acute toxicity (L/EC_{50}) values for the aquatic studies are > 5 mg/l. The T-criterion is considered not to be fulfilled.

Regarding β-caryophyllane the T-screening criterion, based on QSAR data, is fulfilled.

INFORMATION ON USE AND EXPOSURE

Not relevant as the substance is not identified as a PBT.

OTHER INFORMATION

The information and references used in this report were taken from the following sources:

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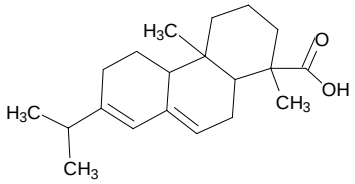
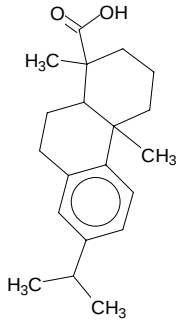
ANNEX

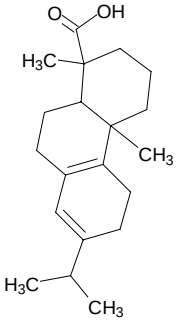
Structural formulas of the substances covered by this assessment. The CAS numbers refer here to the pure substances, not to any resin or rosin acids fraction on fraction on the market.



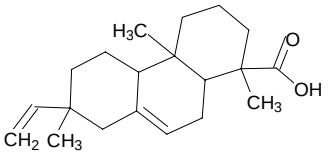
Abietic acid (CAS 514-10-3)



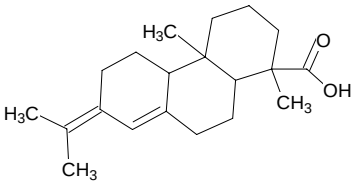
Dehydroabietic acid (CAS 1740-19-8)



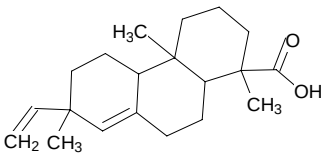
Palustric acid (CAS 1945-53-5)



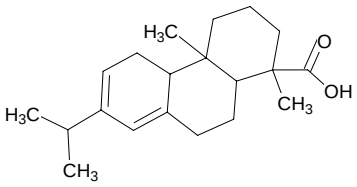
Isopimaric acid (CAS 5835-26-7)



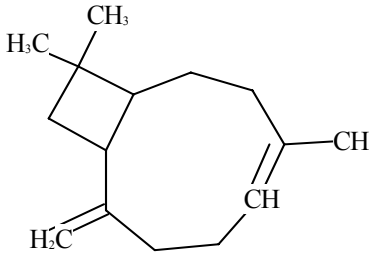
Neoabietic acid (CAS 471-77-2)



Pimaric acid (CAS 127-27-5)



Levopimaric acid (CAS 79-54-9)



Sandaracopimaric acid (CAS 471-74-9)