201-15766B

High Production Volume (HPV) Challenge Program Test Plan and Data Review

Dinonylnaphthalene Category

Melting and Boiling Points

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1; Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2); Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3); Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Remarks Field for Test Substance

Purity of test substances not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

Test conditions were not specified.

Results

CAS No.	Parameter	Value
63512-64-1	Melting point	168.4 ºC
	Boiling point	452.3 ºC
25322-17-2	Melting point	259.5 ºC
	Boiling point	600.4 ºC
57855-77-3	Melting point	261.5 ºC
	Boiling point	604.7 ºC
25619-56-1	Melting point	349.8 ºC
	Boiling point	1124.1 ºC

Conclusions

The data were modeled using the structure activity relationship (SAR) Model MPBPWIN (v1.40) program (1). The model used was received from the U.S. Environmental Protection Agency (EPA).

Remarks Field for Conclusions

The use of these data should be accompanied by a notation that they were modeled using a SAR program rather than based on experimental data.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. U.S. EPA. 2000. Estimation Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software (including the MPBPWIN v1.40 program used to generate these data) are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Vapor Pressure

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1); Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2); Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3); Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Remarks Field for Test Substance

Purity of test substances not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

Test conditions were not specified.

Results

CAS No.	Parameter	Value
63512-64-1	Vapor pressure @ 25 ºC	1.4×10^{-8} mm Hg
25322-17-2	Vapor pressure @ 25 ºC	3.9×10^{-16} mm Hg
57855-77-3	Vapor pressure @ 25 ºC	1.4×10^{-13} mm Hg
25619-56-1	Vapor pressure @ 25 ºC	4.8×10^{-29} mm Hg

Conclusions

These data were modeled using the modified Grain method as applied within the MPBPWIN (v1.40) program (1). The model used was received from the U.S. Environmental Protection Agency (EPA).

Remarks Field for Conclusions

The use of these data should be accompanied by a notation that they were modeled using a SAR program rather than based on experimental data.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software (including the MPBPWIN v1.40 program used to generate these data) are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Water Solubility

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1); Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2); Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3); Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Remarks Field for Test Substance

Purity of test substances not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

Test conditions were not specified.

Results

CAS No.	Parameter	Value
63512-64-1	Water solubility	2.4×10^{-7} mg/L
25322-17-2	Water solubility	2.8×10^{-5} mg/L
57855-77-3	Water solubility	3.1×10^{-7} mg/L
25619-56-1	Water solubility	1.0×10^{-10} mg/L

Conclusions

These data were modeled using the structure activity relationship (SAR) Model WSKOW (v1.41) program (1). The model used was received from the U.S. Environmental Protection Agency (EPA).

Remarks Field for Conclusions

The use of these data should be accompanied by a notation that they were modeled using a SAR program rather than based on experimental data.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software (including the WSKOW v1.41 program used to generate these data) are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Octanol-Water Partition Coefficient (Kow)

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1); Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2); Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3); Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Remarks Field for Test Substance

Purity of test substances not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

Test conditions were not specified.

Results

CAS No.	Parameter	Value
63512-64-1	Kow	11.97
25322-17-2	Kow	9.0
57855-77-3	Kow	10.96
25619-56-1	Kow	23.3

Conclusions

These data were modeled using the structure activity relationship (SAR) Model WSKOW (v1.41) program (1). The model used was received from the U.S. Environmental Protection Agency (EPA).

Remarks Field for Conclusions

The use of these data should be accompanied by a notation that they were modeled using a SAR program rather than based on experimental data.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software (including the WSKOW v1.41 program used to generate these data) are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Stability in Water

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1); Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2); Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3): Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Remarks Field for Test Substance

Purity of test substances not identified.

Method

Method/guideline followed:	Calculated
GLP (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

Test conditions were not specified.

Results

Hydrolysis rate constants cannot be estimated for this category of compounds.

Remarks Field for Results

This category of compounds is resistant to hydrolysis because they lack potentially hydrolysable groups such as alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (1,2).

Conclusions

This category of compounds contains no hydrolysable groups.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Hydrolysis rate constants cannot be estimated for this category of compounds.

References

1. Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods. McGraw Hill, New York, NY.

2. U.S. EPA. 2000. Estimation Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software (including the HYDROWIN v1.67 program) are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Transport Between Environmental Compartments (Fugacity)

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Test Type:	Multimedia (i.e., fugacity) modeling
Model:	EQC (equilibrium criterion) model; version 1.01
GLP Method (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

The EQC model (1, 2) was used for all fugacity calculations as recommended by the U.S. Environmental Protection Agency (EPA). All simulations were conducted at a data temperature of 25°C using default values of the model for compartment dimensions and properties. If chemical-specific data required for the simulations (Table 1) were not available, estimated values were obtained using structure activity relationship (SAR) models, as provided with the EPI Suite™ (v3.11) package (3). Level-I, -II, and -III fugacity models for a Type-1 chemical (i.e., chemical that partitions into all environmental media) were used for the simulations.

Table 1. Physical and chemical properties of diisononylnaphthalene

Property	Value	Comments
Molecular weight (g/mol)	380.7	
Data temperature (ºC)	25	
Water solubility (g/m^3)	2.4×10^{-7}	Estimated value[1]
Log Kow	11.97	Estimated value[2]
Half-life in air (h)	2.9	Estimated value[3]
Half-life in water (h)	1440	Estimated value[3]
Half-life in soil (h)	1440	Estimated value[3]
Half-life in sediment (h)	5760	Estimated value[3]

[1] Water solubility of diisononylnaphthalene at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3).

[2] Log Kow of diisononylnaphthalene at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3).

[3] The overall half-life of diisononylnaphthalene in the various compartments at 25 ºC was estimated using the SAR Models BIOWIN (v4.00) and AOPWIN (v1.90). The models were used as received from the U.S. EPA (3).

Results

Level-I Simulation: A Level-I simulation evaluates the equilibrium distribution of a fixed quantity of chemical in a closed environment with no degradation reactions, no advective processes, and no intermedia transport process (e.g., no wet deposition or sedimentation). Output from the Level-I simulation provides a general indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium.

Results from the Level-I simulation (Table 2) indicate that diisononylnaphthalene has the tendency to partition almost exclusively into the soil compartment, which holds essentially 98% of the total chemical mass. About 2% of the total mass of diisononylnaphthalene is found in the sediment compartment, with an insignificant amount (< 0.1% of the total mass) distributed between the air and water compartments.

Table 2. Environmental distribution of diisononylnaphthalene, based on Level-I fugacity modeling

	Environmental Distribution (%)			
Diisononylnaphthalene	Air	Water	Soil	Sediment
	7.2×10^{-5}	1.2×10^{-7}	97.8	2.2

Level-II Simulation: A Level-II simulation evaluates the equilibrium distribution of a chemical that is continuously discharged to the environment at a constant rate, and achieves a steady-state condition at which the input and output rates are equal. Degradation reactions and advective processes are treated as the mechanism of loss or output. Intermedia transport processes are not quantified (e.g., no wet deposition or sedimentation). Similar to a Level-I simulation, output from a Level-II simulation provides an indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium. In addition, the Level-II simulation also provides an indication of environmental persistence and the loss processes that are likely to be most important.

Results from the Level-II simulation (Table 3) show the same environmental distribution characteristics as the Level-I simulation (Table 2), with 98% of the total mass of diisononylnaphthalene found in the soil compartment. Degradation in air and water and advective losses account for < 0.2% of the total mass removed. Output from the model indicates that diisononylnaphthalene will have a residence time of about 2,111 hours (88 days).

Table 3. Distribution and environmental residence time of diisononylnaphthalene, based on Level-II fugacity modeling

	Environmental Compartment			
Diisononylnaphthalene	Air	Water	Soil	Sediment
• Distribution (%)	7.2×10^{-5}	1.2×10^{-7}	97.8	2.2
• Reaction losses (%)	0.04	1.2×10^{-7}	99.3	0.5
• Advective losses (%)	1.5×10^{-3}	2.5×10^{-7}	ND[1]	0.09
• Overall residence time (h)	2111			
• Reaction residence time (h)	2113			
• Advective residence time (h)	2.3×10^{6}			

[1] ND – Not determined. Value outside the range of the model limits.

Level-III Simulation: A Level-III simulation is similar to a Level-II simulation in that a) the chemical is continuously discharged to the environment at a constant rate, b) it achieves a steady-state condition at which the input and output rates are equal, and c) the mechanism of loss is determined by degradation reactions and advective processes. However, unlike a Level-II simulation, equilibrium between environmental compartments is not assumed and intercompartmental transport processes are quantified (e.g., wet deposition, sedimentation, resuspension, soil runoff, aerosols, etc. are taken into account). Output from a Level-III simulation provides a more realistic description of a chemical's fate, including the important degradation and advective losses and the intermedia transport processes. In addition, the simulation gives an indication of how source of entry of a chemical to the environment (e.g., to air, water, and/or soil) affects distribution and persistence.

Results from the Level-III simulations (Tables 4a-4c) demonstrate that <5% of the total mass of diisononylnaphthalene released into the air or water compartment will be degraded within that compartment. Emission of diisononylnaphthalene directly to air results in 2% of the total chemical mass residing in the air compartment, with degradation in soil and sediment accounting for 76 and 21% respectively of the total mass removed from the local environment (Table 4a). Similar results were obtained when diisononylnaphthalene was released directly to water, with degradation in sediment accounting for 97% of the total mass removed (Table 4b). Emission of diisononylnaphthalene directly to soil results in essentially all of the total chemical mass residing in the soil compartment, with all of the degradation occurring in that compartment (Table 4c). Advective losses of the total chemical mass removed from the system were insignificant (< 0.1%) in most compartments and at most 4% from the air compartment and 18.1 and 10.4% from the water and sediment compartments, respectively. Persistence of diisononylnaphthalene in the model system ranged from 195 to 5,400 hrs, depending on whether the material is emitted to air, soil, or water.

Table 4a. Distribution and environmental residence time of diisononylnaphthalene emitted to the atmospheric compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 1000; Soil = 0; Water = 0				
	Environmental Compartment			
Diisononylnaphthalene	Air	Water	Soil	Sediment
• Distribution (%)	1.9	0.7	76.1	21.3
• Reaction losses (%)	88.3	0.07	7.2	0.5
• Advective losses (%)	3.8	0.1	0	0.1
• Overall residence time (h)	195			
• Reaction residence time (h)	203			
• Advective residence time (h)	4,910			

Table 4b. Distribution and environmental residence time of diisononylnaphthalene emitted to the water compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 0; Soil = 0; Water = 1000				
	Environmental Compartment			
Diisononylnaphthalene	Air	Water	Soil	Sediment
• Distribution (%)	5.1×10^{-8}	3.4	2.0×10^{-6}	96.6
• Reaction losses (%)	6.4×10^{-5}	8.7	5.2×10^{-6}	62.8

• Advective losses (%)	2.7×10^{-6}	18.1	0	10.4
• Overall residence time (h)	5,400			
• Reaction residence time (h)	7,550			
• Advective residence time (h)	18,900			

Table 4c. Distribution and environmental residence time of diisononylnaphthalene emitted to the soil compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 0; Soil = 1000; Water = 0				
	Environmental Compartment			
Diisononylnaphthalene	Air	Water	Soil	Sediment
• Distribution (%)	3.1×10^{-8}	0.002	99.9	0.05
• Reaction losses (%)	1.5×10^{-5}	0.002	100.0	0.01
• Advective losses (%)	6.4×10^{-7}	0.004	0	0.002
• Overall residence time (h)	2,080			
• Reaction residence time (h)	2,080			
• Advective residence time (h)	3.5×10^{7}			

Conclusions

Results from the multimedia model simulations indicate that diisononylnaphthalene will degrade slowly in the environment. If released directly to the air, water and soil compartments simultaneously, 0.05% of the steady-state emission is expected to degrade in air, 2.4% is expected to degrade in water, 29% is expected to partition to and degrade in soil, and 69% is expected to partition to and degrade in sediment. Based on Level-III modeling, it is expected that most of the total steady-state mass of diisononylnaphthalene will reside in the soil and sediment compartments, with a lesser quantity residing in the water compartment and essentially none found in the air.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. Mackay, D.A., A. DiGuardo, S. Paterson, and C.E. Cowan. 1996. Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environm. Toxicol. Chem. 15: 1627-1637.
2. Canadian Environmental Modelling Centre. 2003. EQuilibrium Criterion (EQC) model. Version 2.02. Trent University, Ontario, Canada.
3. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Transport Between Environmental Compartments (Fugacity)

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Test Type:	Multimedia (i.e., fugacity) modeling
Model:	EQC (equilibrium criterion) model; version 1.01
GLP Method (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

The EQC model (1, 2) was used for all fugacity calculations as recommended by the U.S. Environmental Protection Agency (EPA). All simulations were conducted at a data temperature of 25°C using default values of the model for compartment dimensions and properties. If chemical-specific data required for the simulations (Table 1) were not available, estimated values were obtained using structure activity relationship (SAR) models, as provided with the EPI Suite™ (v3.11) package (3). Level-I, -II, and -III fugacity models for a Type-1 chemical (i.e., chemicals that partition into all environmental media) were used for the simulations.

Table 1. Physical and chemical properties of dinonylnaphthalene sulfonic acid

Property	Value	Comments
Molecular weight (g/mol)	460.7	
Data temperature (ºC)	25	
Water solubility (g/m^3)	2.8×10^{-5}	Estimated value[1]
Log Kow	9.0	Estimated value[2]
Half-life in air (h)	7.1	Estimated value[3]
Half-life in water (h)	360	Estimated value[3]
Half-life in soil (h)	360	Estimated value[3]
Half-life in sediment (h)	1440	Estimated value[3]

[1] Water solubility of dinonylnaphthalene sulfonic acid at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3).

[2] Log Kow of dinonylnaphthalene sulfonic acid at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3).

[3] The overall half-life of dinonylnaphthalene sulfonic acid in the various compartments at 25 ºC was estimated using the SAR Models BIOWIN (v4.00) and AOPWIN (v1.90). The models were used as received from the U.S. EPA (3).

Results

Level-I Simulation: A Level-I simulation evaluates the equilibrium distribution of a fixed quantity of chemical in a closed environment with no degradation reactions, no advective processes, and no intermedia transport process (e.g., no wet deposition or sedimentation). Output from the Level-I simulation provides a general indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium.

Results from the Level-I simulation (Table 2) indicate that dinonylnaphthalene sulfonic acid has the tendency to partition almost exclusively into the soil compartment, which holds essentially 98% of the total chemical mass. About 2% of the total mass of dinonylnaphthalene sulfonic acid is found in the sediment compartment, with an insignificant amount (< 0.1% of the total mass) distributed between the air and water compartments.

Table 2. Environmental distribution of dinonylnaphthalene sulfonic acid, based on Level-I fugacity modeling

	Environmental Distribution (%)			
Dinonylnaphthalene sulfonic acid	Air	Water	Soil	Sediment
	4.0×10^{-8}	1.2×10^{-4}	97.8	2.2

Level-II Simulation: A Level-II simulation evaluates the equilibrium distribution of a chemical that is continuously discharged to the environment at a constant rate, and achieves a steady-state condition at which the input and output rates are equal. Degradation reactions and advective processes are treated as the mechanism of loss or output. Intermedia transport processes are not quantified (e.g., no wet deposition or sedimentation). Similar to a Level-I simulation, output from a Level-II simulation provides an indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium. In addition, the Level-II simulation also provides an indication of environmental persistence and the loss processes that are likely to be most important.

Results from the Level-II simulation (Table 3) show the same environmental distribution characteristics as the Level-I simulation (Table 2), with 98% of the total mass of dinonylnaphthalene sulfonic acid found in the soil compartment. Degradation in air and water, and advective losses account for < 0.6% of the total mass removed. Output from the model indicates that dinonylnaphthalene sulfonic acid will have a residence time of about 528 hours (22 days).

Table 3. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid based on Level-II fugacity modeling

	Environmental Compartment			
Dinonylnaphthalene sulfonic acid	Air	Water	Soil	Sediment
• Distribution (%)	4.0×10^{-8}	1.2×10^{-4}	97.8	2.2
• Reaction losses (%)	2.0×10^{-6}	1.2×10^{-4}	99.4	0.6
• Advective losses (%)	2.1×10^{-7}	6.4×10^{-5}	ND[1]	0.02
• Overall residence time (h)	528			
• Reaction residence time (h)	528			

• Advective residence time (h)	2.3 x 10^6

[1]ND – Not determined. Value outside the range of the model limits.

Level-III Simulation: A Level-III simulation is similar to a Level-II simulation in that a) the chemical is continuously discharged to the environment at a constant rate, b) it achieves a steady-state condition at which the input and output rates are equal, and c) the mechanism of loss is determined by degradation reactions and advective processes. However, unlike a Level-II simulation, equilibrium between environmental compartments is not assumed and intercompartmental transport processes are quantified (e.g., wet deposition, sedimentation, resuspension, soil runoff, aerosols, etc. are taken into account). Output from a Level-III simulation provides a more realistic description of a chemical's fate, including the important degradation and advective losses and the intermedia transport processes. In addition, the simulation gives an indication of how source of entry of a chemical to the environment (e.g., to air, water, and/or soil) affects distribution and persistence.

Results from the Level-III simulations (Tables 4a-4c) demonstrate that <10% of the total mass of dinonylnaphthalene sulfonic acid released into the air or water compartment will be degraded within that compartment. Emission of dinonylnaphthalene sulfonic acid directly to air results in 5% of the total chemical mass residing in the air compartment, with degradation in soil and sediment accounting for 74 and 19%, respectively, of the total mass removed from the local environment (Table 4a). When dinonylnaphthalene sulfonic acid was released directly to water, degradation in sediment accounts for 90% of the total mass removed (Table 4b). Emission of dinonylnaphthalene sulfonic acid directly to soil results in essentially all of the total chemical mass residing in the soil compartment, with all of the degradation occurring in that compartment (Table 4c). Advective losses of the total chemical mass removed from the system were insignificant (< 0.1%) in most compartments, and at most 7% from the air compartment and 14% from the water compartment. Persistence of dinonylnaphthalene sulfonic acid in the model system ranged from 139 to 1,340 hrs, depending on whether the material is emitted to air, soil, or water.

Table 4a. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid emitted to the atmospheric compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 1000; Soil = 0; Water = 0				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid	Air	Water	Soil	Sediment
• Distribution (%)	5.3	2.1	73.7	19.0
• Reaction losses (%)	70.8	0.6	19.7	1.3
• Advective losses (%)	7.3	0.3	0	0.05
• Overall residence time (h)	139			
• Reaction residence time (h)	150			
• Advective residence time (h)	1,820			

Table 4b. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid emitted to the water compartment, based on Level-III fugacity modeling.

Emission Rates (kg/h): Air = 0; Soil = 0; Water = 1000				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid	Air	Water	Soil	Sediment
• Distribution (%)	3.5×10^{-8}	10.1	4.9×10^{-7}	89.9
• Reaction losses (%)	4.5×10^{-6}	26.1	1.3×10^{-6}	57.9
• Advective losses (%)	4.6×10^{-7}	13.6	0	2.4
• Overall residence time (h)	1,340			
• Reaction residence time (h)	1,590			
• Advective residence time (h)	8,370			

Table 4c. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid emitted to the soil compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 0; Soil = 1000; Water = 0				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid	Air	Water	Soil	Sediment
• Distribution (%)	1.5×10^{-9}	0.001	100.0	0.01
• Reaction losses (%)	7.5×10^{-8}	0.001	100.0	0.003
• Advective losses (%)	7.7×10^{-9}	0.0007	0	0.0001
• Overall residence time (h)	520			
• Reaction residence time (h)	520			
• Advective residence time (h)	6.3×10^{7}			

Conclusions

Results from the multimedia model simulations indicate that dinonylnaphthalene sulfonic acid will degrade slowly in the environment. If released directly to the air, water, and soil compartments simultaneously, 0.4% of the steady-state emission is expected to degrade in air, 7% is expected to degrade in water, 31% is expected to partition to and degrade in soil, and 62% is expected to partition to and degrade in sediment. Based on Level-III modeling, it is expected that >92% of the total steady-state mass of dinonylnaphthalene sulfonic acid will reside in the sediment and soil compartments, with a lesser quantity residing in the water compartment and very little found in the air.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. Mackay, D.A., A. DiGuardo, S. Paterson, and C.E. Cowan. 1996. Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environm. Toxicol. Chem. 15: 1627-1637.
2. Canadian Environmental Modelling Centre. 2003. EQuilibrium Criterion (EQC) model. Version 2.02. Trent University, Ontario, Canada.
3. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Transport Between Environmental Compartments (Fugacity)

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Test Type:	Multimedia (i.e., fugacity) modeling
Model:	EQC (equilibrium criterion) model; version 1.01
GLP Method (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

The EQC model (1, 2) was used for all fugacity calculations as recommended by the U.S. Environmental Protection Agency (EPA). All simulations were conducted at a data temperature of 25°C using default values of the model for compartment dimensions and properties. If chemical-specific data required for the simulations (Table 1) were not available, estimated values were obtained using structure activity relationship (SAR) models, as provided with the EPI Suite™ (v3.11) package (3). Level-I, -II, and -III fugacity models for a Type-1 chemical (i.e., chemicals that partition into all environmental media) were used for the simulations.

Table 1. Physical and chemical properties of dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Property	Value	Comments
Molecular weight (g/mol)	500.8	
Data temperature (ºC)	25	
Water solubility (g/m^3)	3.1×10^{-7}	Estimated value[1]
Log Kow	10.96	Estimated value[2]
Half-life in air (h)	7.2	Estimated value[3]
Half-life in water (h)	900	Estimated value[3]
Half-life in soil (h)	900	Estimated value[3]
Half-life in sediment (h)	3600	Estimated value[3]

[1] Water solubility of dinonylnaphthalene sulfonic acid, calcium salt at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3).

[2] Log Kow of dinonylnaphthalene sulfonic acid, calcium salt at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3).

[3] The overall half-life of dinonylnaphthalene sulfonic acid, calcium salt in the various compartments at 25 ºC was estimated using the SAR Models BIOWIN (v4.00) and AOPWIN (v1.90). The models were used as received from the U.S. EPA (3).

Results

Level-I Simulation: A Level-I simulation evaluates the equilibrium distribution of a fixed quantity of chemical in a closed environment with no degradation reactions, no advective processes, and no intermedia transport process (e.g., no wet deposition or sedimentation). Output from the Level-I simulation provides a general indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium.

Results from the Level-I simulation (Table 2) indicate that dinonylnaphthalene sulfonic acid, calcium salt has the tendency to partition almost exclusively into the soil compartment, which holds essentially 98% of the total chemical mass. About 2% of the total mass of dinonylnaphthalene sulfonic acid, calcium salt is found in the sediment compartment, with an insignificant amount (< 0.1% of the total mass) distributed between the air and water compartments.

Table 2. Environmental distribution of dinonylnaphthalene sulfonic acid, calcium salt, based on Level-I fugacity modeling

Dinonylnaphthalene sulfonic acid, calcium salt	Environmental Distribution (%)			
	Air	Water	Soil	Sediment
	3.9×10^{-9}	1.2×10^{-6}	97.8	2.2

Level-II Simulation: A Level-II simulation evaluates the equilibrium distribution of a chemical that is continuously discharged to the environment at a constant rate, and achieves a steady-state condition at which the input and output rates are equal. Degradation reactions and advective processes are treated as the mechanism of loss or output. Intermedia transport processes are not quantified (e.g., no wet deposition or sedimentation). Similar to a Level-I simulation, output from a Level-II simulation provides an indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium. In addition, the Level-II simulation also provides an indication of environmental persistence and the loss processes that are likely to be most important.

Results from the Level-II simulation (Table 3) show the same environmental distribution characteristics as the Level-I simulation (Table 2), with 98% of the total mass of dinonylnaphthalene sulfonic acid, calcium salt found in the soil compartment. Degradation in air and water, and advective losses account for < 0.1% of the total mass removed. Output from the model indicates that dinonylnaphthalene sulfonic acid, calcium salt will have a residence time of 1,320 hours (55 days).

Table 3. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, calcium salt, based on Level-II fugacity modeling

	Environmental Compartment			
Dinonylnaphthalene sulfonic acid,	Air	Water	Soil	Sediment

calcium salt				
• Distribution (%)	3.9×10^{-9}	1.2×10^{-6}	97.8	2.2
• Reaction losses (%)	5.0×10^{-7}	1.2×10^{-6}	99.4	0.6
• Advective losses (%)	5.2×10^{-8}	1.6×10^{-6}	ND[1]	0.06
• Overall residence time (h)	1,320			
• Reaction residence time (h)	1,321			
• Advective residence time (h)	2.3×10^{6}			

[1]ND – Not determined. Value outside the range of the model limits.

Level-III Simulation: A Level-III simulation is similar to a Level-II simulation in that a) the chemical is continuously discharged to the environment at a constant rate, b) it achieves a steady-state condition at which the input and output rates are equal, and c) the mechanism of loss is determined by degradation reactions and advective processes. However, unlike a Level-II simulation, equilibrium between environmental compartments is not assumed and intercompartmental transport processes are quantified (e.g., wet deposition, sedimentation, resuspension, soil runoff, aerosols, etc. are taken into account). Output from a Level-III simulation provides a more realistic description of a chemical's fate, including the important degradation and advective losses and the intermedia transport processes. In addition, the simulation gives an indication of how source of entry of a chemical to the environment (e.g., to air, water, and/or soil) effects distribution and persistence.

Results from the Level-III simulations (Tables 4a-4c) demonstrate that <5% of the total mass of dinonylnaphthalene sulfonic acid, calcium salt released into the air or water compartment will be degraded within that compartment. Emission of dinonylnaphthalene sulfonic acid, calcium salt directly to air results in 2.2% of the total chemical mass residing in the air compartment, with degradation in soil and sediment accounting for 75 and 21%, respectively, of the total mass removed from the local environment (Table 4a). When dinonylnaphthalene sulfonic acid, calcium salt was released directly to water, degradation in sediment accounted for 95% of the total mass removed (Table 4b). Emission of dinonylnaphthalene sulfonic acid, calcium salt directly to soil results in essentially all of the total chemical mass residing in the soil compartment, with all of the degradation occurring in that compartment (Table 4c). Advective losses of the total chemical mass removed from the system were insignificant (< 0.1%) in most compartments, and at most 7% from the air compartment and 17% from the water compartment. Persistence of dinonylnaphthalene sulfonic acid, calcium salt in the model system ranged from 340 to 3,480 hrs, depending on whether the material is emitted to air, soil, or water.

Table 4a. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, calcium salt emitted to the atmospheric compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 1000; Soil = 0; Water = 0				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, calcium salt	Air	Water	Soil	Sediment
• Distribution (%)	2.2	1.1	75.4	21.4
• Reaction losses (%)	70.8	0.3	19.7	1.4
• Advective losses (%)	7.3	0.4	0	0.1

• Overall residence time (h)	340
• Reaction residence time (h)	369
• Advective residence time (h)	4,350

Table 4b. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, calcium salt emitted to the water compartment, based on Level-III fugacity modeling.

Emission Rates (kg/h): Air = 0; Soil = 0; Water = 1000				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, calcium salt	Air	Water	Soil	Sediment
• Distribution (%)	1.8×10^{-9}	4.8	6.3×10^{-8}	95.2
• Reaction losses (%)	6.1×10^{-7}	12.8	1.7×10^{-7}	63.8
• Advective losses (%)	6.3×10^{-8}	16.7	0	6.6
• Overall residence time (h)	3,480			
• Reaction residence time (h)	4,540			
• Advective residence time (h)	14,900			

Table 4c. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, calcium salt emitted to the soil compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 0; Soil = 1000; Water = 0				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, calcium salt	Air	Water	Soil	Sediment
• Distribution (%)	3.7×10^{-11}	0.002	100.0	0.03
• Reaction losses (%)	4.6×10^{-9}	0.002	100.0	0.008
• Advective losses (%)	4.7×10^{-10}	0.002	0	0.0009
• Overall residence time (h)	1,300			
• Reaction residence time (h)	1,300			
• Advective residence time (h)	4.3×10^{7}			

Conclusions

Results from the multimedia model simulations indicate that dinonylnaphthalene sulfonic acid, calcium salt will degrade slowly in the environment. If released directly to the air, water, and soil compartments simultaneously, 0.14% of the steady-state emission is expected to degrade in air, 3.3% is expected to degrade in water, 30% is expected to partition to and degrade in soil, and 66% expected to partition to and degrade in sediment. Based on Level-III modeling, it is expected that >96% of the total steady-state mass of dinonylnaphthalene sulfonic acid, calcium salt will reside in the sediment and soil compartments, with a lesser quantity residing in the water compartment and very little found in the air.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. Mackay, D.A., A. DiGuardo, S. Paterson, and C.E. Cowan. 1996. Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environm. Toxicol. Chem. 15: 1627-1637.
2. Canadian Environmental Modelling Centre. 2003. EQuilibrium Criterion (EQC) model. Version 2.02. Trent University, Ontario, Canada.
3. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Transport Between Environmental Compartments (Fugacity)

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Remarks Field for Test Substance

Purity of test substance not identified.

Method

Test Type:	Multimedia (i.e., fugacity) modeling
Model:	EQC (equilibrium criterion) model; version 1.01
GLP Method (Y/N):	No
Year (study performed):	2004

Remarks Field for Test Conditions

The EQC model (1, 2) was used for all fugacity calculations as recommended by the U.S. Environmental Protection Agency (EPA). All simulations were conducted at a data temperature of 25°C using default values of the model for compartment dimensions and properties. If chemical-specific data required for the simulations (Table 1) were not available, estimated values were obtained using structure activity relationship (SAR) models, as provided with the EPI Suite™ (v3.11) package (3). Level-I, -II, and -III fugacity models for a Type-1 chemical (i.e., chemicals that partition into all environmental media) were used for the simulations.

Table 1. Physical and chemical properties of dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Property	Value	Comments
Molecular weight (g/mol)	1056.8	
Data temperature (ºC)	25	
Water solubility (g/m^3)	1.0×10^{-10}	Estimated value[1]
Log Kow	23.3	Estimated value[2]
Half-life in air (h)	3.6	Estimated value[3]
Half-life in water (h)	1440	Estimated value[3]
Half-life in soil (h)	1440	Estimated value[3]
Half-life in sediment (h)	5760	Estimated value[3]

[1] Water solubility of dinonylnaphthalene sulfonic acid, barium salt at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3). The input range maximum of 1.0×10^{-10} was applied in the EQC model for Level I and II simulations.

[2] Log Kow of dinonylnaphthalene sulfonic acid, barium salt at 25 ºC was estimated using the SAR Model WSKOWWIN (v1.40). The model was used as received from the U.S. EPA (3). The input range maximum of 12 was applied in the EQC model for Level I and II simulations.

[3] The overall half-life of dinonylnaphthalene sulfonic acid, barium salt in the various compartments at 25 ºC was estimated using the SAR Models BIOWIN (v4.00) and AOPWIN (v1.90). The models were used as received from the U.S. EPA (3).

Results

Level-I Simulation: A Level-I simulation evaluates the equilibrium distribution of a fixed quantity of chemical in a closed environment with no degradation reactions, no advective processes, and no intermedia transport process (e.g., no wet deposition or sedimentation). Output from the Level-I simulation provides a general indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium.

Results from the Level-I simulation (Table 2) indicate that dinonylnaphthalene sulfonic acid, barium salt has the tendency to partition almost exclusively into the soil compartment, which holds essentially 98% of the total chemical mass. About 2% of the total mass of dinonylnaphthalene sulfonic acid, barium salt is found in the sediment compartment, with an insignificant (<0.1% of the total mass) distributed between the air and water compartments.

Table 2. Environmental distribution of dinonylnaphthalene sulfonic acid, barium salt, based on Level-I fugacity modeling

Dinonylnaphthalene sulfonic acid, barium salt	Environmental Distribution (%)			
	Air	Water	Soil	Sediment
	2.4×10^{-5}	1.1×10^{-7}	97.8	2.2

Level-II Simulation: A Level-II simulation evaluates the equilibrium distribution of a chemical that is continuously discharged to the environment at a constant rate, and achieves a steady-state condition at which the input and output rates are equal. Degradation reactions and advective processes are treated as the mechanism of loss or output. Intermedia transport processes are not quantified (e.g., no wet deposition or sedimentation). Similar to a Level-I simulation, output from a Level-II simulation provides an indication of the likely media into which a chemical will tend to partition and the relative concentrations in each medium. In addition, the Level-II simulation also provides an indication of environmental persistence and the loss processes that are likely to be most important.

Results from the Level-II simulation (Table 3) show the same environmental distribution characteristics as the Level-I simulation (Table 2), with 98% of the total mass of dinonylnaphthalene sulfonic acid, barium salt found in the soil compartment. Degradation in air and water, and advective losses account for < 0.1% of the total mass removed. Output from the model indicates that dinonylnaphthalene sulfonic acid, barium salt will have a residence time of 2112 hours (88 days).

Table 3. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, barium salt, based on Level-II fugacity modeling

	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, barium salt	Air	Water	Soil	Sediment

• Distribution (%)	2.4×10^{-5}	1.1×10^{-7}	97.8	2.2
• Reaction losses (%)	9.6×10^{-3}	1.1×10^{-7}	99.3	0.6
• Advective losses (%)	5.0×10^{-4}	2.3×10^{-7}	ND[1]	0.09
• Overall residence time (h)	2112			
• Reaction residence time (h)	2114			
• Advective residence time (h)	2.3×10^{6}			

[1]ND – Not determined. Value outside the range of the model limits.

Level-III Simulation: A Level-III simulation is similar to a Level-II simulation in that a) the chemical is continuously discharged to the environment at a constant rate, b) it achieves a steady-state condition at which the input and output rates are equal, and c) the mechanism of loss is determined by degradation reactions and advective processes. However, unlike a Level-II simulation, equilibrium between environmental compartments is not assumed and intercompartmental transport processes are quantified (e.g., wet deposition, sedimentation, resuspension, soil runoff, aerosols, etc. are taken into account). Output from a Level-III simulation provides a more realistic description of a chemical's fate, including the important degradation and advective losses and the intermedia transport processes. In addition, the simulation gives an indication of how source of entry of a chemical to the environment (e.g., to air, water, and/or soil) effects distribution and persistence.

Results from the Level-III simulations (Tables 4a-4c) demonstrate that <2% of the total mass of dinonylnaphthalene sulfonic acid, barium salt released into the air or water compartment will be degraded within that compartment. Emission of dinonylnaphthalene sulfonic acid, barium salt directly to air results in 1.4% of the total chemical mass residing in the air compartment, with degradation in soil and sediment accounting for 77 and 21%, respectively, of the total mass removed from the local environment (Table 4a). When dinonylnaphthalene sulfonic acid, barium salt was released directly to water, degradation in sediment accounts for 97% of the total mass removed (Table 4b). Emission of dinonylnaphthalene sulfonic acid, barium salt directly to soil results in essentially all of the total chemical mass residing in the soil compartment, with all of the degradation occurring in that compartment. Advective losses of the total chemical mass removed from the system were insignificant (< 0.1%) in most compartments, and at most 4% from the air compartment and 18% from the water compartment. Persistence of dinonylnaphthalene sulfonic acid, barium salt in the model system ranged from 314 to 5,400 hrs, depending on whether the material is emitted to air, soil, or water.

Table 4a. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, barium salt emitted to the atmospheric compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 1000; Soil = 0; Water = 0				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, barium salt	Air	Water	Soil	Sediment
• Distribution (%)	1.4	0.7	76.5	21.4
• Reaction losses (%)	82.9	0.1	11.6	0.8
• Advective losses (%)	4.3	0.2	0	0.1
• Overall residence time (h)	314			
• Reaction residence time (h)	329			

• Advective residence time (h)	6,750

Table 4b. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, barium salt emitted to the water compartment, based on Level-III fugacity modeling.

Emission Rates (kg/h): Air = 0; Soil = 0; Water = 1000				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, barium salt	Air	Water	Soil	Sediment
• Distribution (%)	5.7×10^{-22}	3.4	3.2×10^{-20}	96.6
• Reaction losses (%)	6.0×10^{-19}	8.7	8.3×10^{-20}	62.8
• Advective losses (%)	3.1×10^{-20}	18.1	0	10.4
• Overall residence time (h)	5,400			
• Reaction residence time (h)	7,550			
• Advective residence time (h)	18,900			

Table 4c. Distribution and environmental residence time of dinonylnaphthalene sulfonic acid, barium salt emitted to the soil compartment, based on Level-III fugacity modeling

Emission Rates (kg/h): Air = 0; Soil = 1000; Water = 0				
	Environmental Compartment			
Dinonylnaphthalene sulfonic acid, barium salt	Air	Water	Soil	Sediment
• Distribution (%)	1.1×10^{-23}	0.002	99.9	0.05
• Reaction losses (%)	4.5×10^{-21}	0.002	100.0	0.01
• Advective losses (%)	2.3×10^{-22}	0.004	0	0.002
• Overall residence time (h)	2,080			
• Reaction residence time (h)	2,080			
• Advective residence time (h)	3.5×10^{7}			

Conclusions

Results from the multimedia model simulations indicate that dinonylnaphthalene sulfonic acid, barium salt will degrade slowly in the environment. If released directly to the air, water, and soil compartments simultaneously, 0.05% of the steady-state emission is expected to degrade in air, 2.4% is expected to degrade in water, 30% is expected to partition to and degrade in soil, and 68% expected to partition to and degrade in sediment. Based on Level-III modeling, it is expected that >98% of the total steady-state mass of dinonylnaphthalene sulfonic acid, barium salt will reside in the sediment and soil compartments, with a lesser quantity residing in the water compartment and very little found in the air.

Data Quality

Reliabilities (Klimisch Code): 2. (Valid with restrictions)

Remarks Field for Data Reliability

Data were modeled rather than based on experimental results.

References

1. Mackay, D.A., A. DiGuardo, S. Paterson, and C.E. Cowan. 1996. Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environm. Toxicol. Chem. 15: 1627-1637.
2. Canadian Environmental Modelling Centre. 2003. EQuilibrium Criterion (EQC) model. Version 2.02. Trent University, Ontario, Canada.
3. U.S. EPA. 2000. Estimations Programs Interface (EPI) Suite, Version 3.11. The EPI Suite™ and the individual models included within the software are owned and copyright protected by the U.S. EPA.

Other

Last changed (administrative field for updating): 12/21/04

Acute Oral Toxicity

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Rat/Wistar
Sex:	Male
No. of animals per dose group:	10
Vehicle:	Not applicable; test substance dose undiluted
Route of Administration:	Oral via gastric intubation (gavage)

Remarks Field for Test Conditions

Each rat received a single dose of the test substance. Young rats weighing 200 to 300 g were used in the study. The rats were fasted for 18 hours prior to test substance administration and received a single dose of 5,000 mg/kg body weight of undiluted test substance. The rats were individually housed and observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was >5,000 mg/kg for male rats evaluated in the study. There were no signs of gross toxicity. An autopsy of the single mortality revealed liver discoloration, stomach distension, and possible lung and stomach hemorrhage.

Conclusions

The acute oral LD_{50} for the test material was >5,000 mg/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-402

Other

Last changed (administrative field for updating): 12/21/04

Acute Oral Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Sprague Dawley albino rats
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Aliphatic hydrocarbon
Route of Administration:	Oral via gastric intubation (gavage)

Remarks Field for Test Conditions

Each rat received a single dose of the test substance in aliphatic hydrocarbon diluent oil. Young rats weighing 200 to 300 g were used in the study. The rats were fasted for 18 hours prior to test substance administration and received a single dose of 5,000 mg/kg body weight of test substance in aliphatic hydrocarbon diluent oil. The rats were individually housed and observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was >5,000 mg/kg for the male and female rats evaluated in the study. There were no signs of gross toxicity. An autopsy of the single mortality revealed gastrointestinal bloat.

Conclusions

The acute oral LD_{50} for the test material was >5,000 mg/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-293

Other

Last changed (administrative field for updating): 12/21/04

Acute Oral Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Sprague Dawley albino rats
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Diluent oil
Route of Administration:	Oral via gastric intubation (gavage)

Remarks Field for Test Conditions

Each rat received a single dose of the test substance in diluent oil. Young rats weighing 200 to 300 g were used in the study. The rats were fasted for 18 hours prior to test substance administration and received a single dose of 5,000 mg/kg body weight of test substance in diluent oil. The rats were individually housed and observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was >5,000 mg/kg for male and female rats evaluated in the study. There were no signs of gross toxicity. All animals appeared active and healthy. An autopsy of the single mortality was unremarkable.

Conclusions

The acute oral LD_{50} for the test material was >5,000 mg/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-357

Other

Last changed (administrative field for updating): 12/21/04

Acute Oral Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Rat/Wistar
Sex:	Male
No. of animals per dose group:	10
Vehicle:	Diluent oil
Route of Administration:	Oral via gastric intubation (gavage)

Remarks Field for Test Conditions

Each rat received a single dose of the test substance in diluent oil. Young rats weighing 200 to 300 g were used in the study. The rats were fasted for 18 hours prior to test substance administration and received a single dose of 5,000 mg/kg body weight of test substance in diluent oil. The rats were individually housed and observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was <5,000 mg/kg for male rats evaluated in the study. There were no signs of gross toxicity. Seven rats died during the 14-day study period. The autopsies were unremarkable. Possible intestinal hemorrhage and liver enlargement were seen in one subject.

Conclusions

The acute oral LD_{50} for the test material was <5,000 mg/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-399

Other

Last changed (administrative field for updating): 12/21/04

Acute Oral Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1980
Species/Strain:	Rat/Wistar
Sex:	Male and female
No. of animals per dose group:	25 per sex
Vehicle:	Diluent oil
Route of Administration:	Oral via gastric intubation (gavage)

Remarks Field for Test Conditions

The rats were fasted for 18 hours prior to test substance administration and each rat received a single dose of the test substance in diluent oil. Young rats weighing 200 to 300 g were exposed in groups of 5 per sex to concentrations of 2, 3, 4, 5, and 6 mL/kg. The rats were observed for 14 days. Food and water were provided *ad-libitum*.

Results

The results for the study are summarized in Table 1. The acute median lethal dose (LD_{50}) for the test material was 3.5 mL/kg, with 95% confidence limits of 2.8 to 4.3 mL/kg. The LD_{50} was computed by the Litchfield-Wilcoxin method of probit analysis. Results observed during autopsy included lung hemorrhage, discolored spleen, liver discoloration, stomach hemorrhage, subcutaneous hemorrhage, gastrointestinal hemorrhage, bloated stomach, and ocular hemorrhage.

Table 1: Number of deaths at each dose level

Sex	Dose Level (mL/kg)	# Deaths	Days to Death
Males	2	0/5	---
	3	1/5	4
	4	3/5	2, 2, 3
	5	2/5	2,5
	6	5/5	2, 2, 2, 3, 6
Females	2	2/5	2, 10
	3	2/5	2, 3
	4	3/5	2, 3, 5
	5	4/5	2, 3, 3, 5
	6	4/5	2, 3, 5, 5

Conclusions

The acute oral LD_{50} for the test material was 3.5 mL/kg.

Data Quality

Reliabilities (Klimisch Code): 1. (Reliable without restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-467

Other

Last changed (administrative field for updating): 12/21/04

Acute Oral Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Modified Federal Hazardous Substances Act (FHSA), 16 CFR 1500
GLP (Y/N):	No
Year (study performed):	1981
Species/Strain:	Rat/Sprague Dawley
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Diluent oil
Route of Administration:	Oral via food consumption

Remarks Field for Test Conditions

The rats were fasted for 18 hours prior to test substance administration. The test material was mixed with diluent oil and subsequently with ground rat chow. The time required to consume the entire amount of test material was recorded. Young rats weighing 200 to 300 g were exposed to test material equivalent to 5.0 g/kg body weight. The rats were observed for 14 days. Food and water were provided *ad-libitum* after the test material was consumed.

Results

The acute median lethal dose (LD_{50}) for the test material is >5.0 g/kg when ingested orally in food. All rats appeared healthy and active throughout the 14-day test period.

Conclusions

The acute oral LD_{50} for the test material was >5,000 mg/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-1438

Other

Last changed (administrative field for updating): 12/21/04

Acute Inhalation Toxicity

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Rat/Wistar
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Not applicable; test substance dose undiluted
Route of Administration:	Inhalation (aerosol)

Remarks Field for Test Conditions

The rats received a single exposure to the aerosolized test substance in an inhalation chamber. The duration of the exposure was 1 hour. The spray was introduced into the chamber via a nebulizer and directed away from the animals. The chamber was saturated with 17 mg/L of the test material.

Results

The acute median lethal concentration (LC_{50}) for the test material was >17 mg/L for male and female rats evaluated in the study. There were no signs of clinical effects or gross toxicity.

Conclusions

The acute inhalation LC_{50} for the test material was >17 mg/L.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-381

Other

Last changed (administrative field for updating): 12/21/04

Acute Inhalation Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1977
Species/Strain:	Rat/Wistar
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Aliphatic hydrocarbon
Route of Administration:	Inhalation (aerosol)

Remarks Field for Test Conditions

The rats received a single exposure to the aerosolized test material in aliphatic hydrocarbon in an inhalation chamber. The duration of the exposure was 1 hour. The spray was introduced into the chamber via a nebulizer, was circulated, and was directed away from the animals. The chamber was saturated with 200 mg/L of the test material in aliphatic hydrocarbon prior to the period of exposure. The rats were observed for 14 days following exposure.

Results

The acute median lethal concentration (LC_{50}) for the test material was >200 mg/L for male and female rats evaluated in the study. There were no untoward reactions or gross toxicity during the 14-day observation period.

Conclusions

The acute inhalation LC_{50} for the test material was >200 mg/L.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-307

Other

Last changed (administrative field for updating): 12/21/04

Acute Inhalation Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Rat/Wistar
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Diluent oil
Route of Administration:	Inhalation (aerosol)

Remarks Field for Test Conditions

The rats, 200 to 300 g size, were exposed to the test material in diluent oil, vaporized in an inhalation chamber for 1 hour. The chamber was saturated with 18 mg/L nominal of the test material prior to the period of exposure. The rats were observed for 14 days following exposure. Food and water were provided *ad-libitum*.

Results

The acute median lethal concentration (LC_{50}) for the test material was >18 mg/L for male and female rats evaluated in the study. There were no signs of clinical effects or gross toxicity.

Conclusions

The acute inhalation LC_{50} for the test material was >18 mg/L.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-350

Other

Last changed (administrative field for updating): 12/21/04

Acute Inhalation Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	Rat/Wistar
Sex:	Male and female
No. of animals per dose group:	5 per sex
Vehicle:	Diluent oil
Route of Administration:	Inhalation (aerosol)

Remarks Field for Test Conditions

The rats were exposed to an aerosol of the test material in diluent oil in an inhalation chamber for 1 hour. The spray was introduced into the chamber via a nebulizer and directed away from the animals. The chamber was saturated with 21 mg/L of the test material.

Results

The acute median lethal concentration (LC_{50}) for the test material was >21 mg/L for male and female rats evaluated in the study. There were no signs of clinical effects or gross toxicity.

Conclusions

The acute inhalation LC_{50} for the test material was >21 mg/L.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-378

Other

Last changed (administrative field for updating): 12/21/04

Acute Dermal Toxicity

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbit
Sex:	Male and female
No. of animals per dose group:	2 male, 3 female
Vehicle:	Not applicable; test substance dose undiluted
Route of Administration:	Dermal application

Remarks Field for Test Conditions

Each rabbit was prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 5 to 6 cm^2 area on two males and three females. A patch containing 20 g/kg body weight of the test material was placed over a 5 to 6 cm^2 area on all rabbits and secured with an elastic sleeve. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages. The rabbits were observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was >20 g/kg for male and female rabbits evaluated in the study. Clinical results included subtle reversible anorexia.

Conclusions

The acute dermal LD_{50} for the test material was >20 g/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-410

Other

Last changed (administrative field for updating): 12/21/04

Acute Dermal Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1977
Species/Strain:	New Zealand albino rabbit
Sex:	Not defined
No. of animals per dose group:	10
Vehicle:	Kerosene
Route of Administration:	Dermal application

Remarks Field for Test Conditions

The test material, diluted in kerosene, was applied at a dose of 2 g/kg to the moistened clipped skin of 10 rabbits (5 intact and 5 abraded). The rabbits were then wrapped with a rubber dam. After 24 hours, the rubber dam was removed and the residue gently washed off. The test site was examined for erythema and edema, and scores were recorded for 14 days. Body weights were recorded on Days 0 and 14. Rabbits were observed daily for signs of toxicity. All surviving animals were sacrificed at 14 days after treatment and necropsied.

Results

The acute median lethal dose (LD_{50}) for the test material was >2 g/kg for rabbits evaluated in the study. All animals appeared normal and gained weight during the study. There were no signs of gross pathology.

Conclusions

The acute dermal LD_{50} for the test material was >2 g/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Huntingdon Life Sciences Study No. 777-281

Other

Last changed (administrative field for updating): 12/21/04

Acute Dermal Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1977
Species/Strain:	New Zealand albino rabbit
Sex:	Not defined
No. of animals per dose group:	10
Vehicle:	Aliphatic hydrocarbon
Route of Administration:	Dermal application

Remarks Field for Test Conditions

The test material, diluted in aliphatic hydrocarbon, was applied at a dose of 2 g/kg to the moistened clipped skin of 10 rabbits (5 intact and 5 abraded). The rabbits were then wrapped with a rubber dam. After 24 hours, the rubber dam was removed and the residue gently washed off. The test site was examined for erythema and edema, and scores were recorded daily for 14 days. Body weights were recorded on Days 0 and 14. Rabbits were observed daily for signs of toxicity. All surviving animals were sacrificed at 14 days after treatment and necropsied.

Results

The acute median lethal dose (LD_{50}) for the test material was >2 g/kg for the rabbits evaluated in the study. All animals appeared normal and gained weight during the study. There were no signs of gross pathology.

Conclusions

The acute dermal LD_{50} for the test material was >2 g/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Huntingdon Life Sciences, Study No. 777-282

Other

Last changed (administrative field for updating): 12/21/04

Acute Dermal Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Male and female
No. of animals per dose group:	2 male, 3 female
Vehicle:	Diluent oil
Route of Administration:	Dermal application

Remarks Field for Test Conditions

Each rabbit was prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 5 to 6 cm^2 area on two males and three females. A patch containing 20 g/kg body weight of the test material in diluent oil was placed over a 5 to 6 cm^2 area on all rabbits and secured with an elastic sleeve. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages. The rabbits were observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was >20 g/kg for male and female rabbits evaluated in the study. Clinical results included anorexia for the first 5 days, and some weight loss that reversed after 9 days.

Conclusions

The acute dermal LD_{50} for the test material was >20 g/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-346

Other

Last changed (administrative field for updating): 12/21/04

Acute Dermal Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Male and female
No. of animals per dose group:	2 male, 3 female
Vehicle:	Diluent oil
Route of Administration:	Dermal application

Remarks Field for Test Conditions

Each rabbit was prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 5 to 6 cm^2 area on two males and three females. A patch containing 20 g/kg body weight of the test material in diluent oil was placed over a 5 to 6 cm^2 area on all rabbits and secured with an elastic sleeve. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages. The rabbits were observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was <20 g/kg for male and female rabbits evaluated in the study. Eight of the 10 rabbits exposed to the test material died during the study. Rabbits exhibited ataxia, debilitation, anorexia, and weight loss. Autopsies revealed hepatic discoloration.

Conclusions

The acute dermal LD_{50} for the test material was <20 g/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-407

Other

Last changed (administrative field for updating): 12/21/04

Acute Dermal Toxicity

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1981
Species/Strain:	New Zealand albino rabbits
Sex:	Male and female
No. of animals per dose group:	2 male, 3 female
Vehicle:	Naphthenic diluent oil
Route of Administration:	Dermal application

Remarks Field for Test Conditions

Each rabbit was prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 5 to 6 cm^2 area on two males and three females. A patch containing 2.0 mL/kg body weight of the test material in naphthenic diluent oil was placed over a 4 to 5 cm^2 area on all rabbits and secured with tape and an elastic sleeve. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages. The rabbits were observed for 14 days. Food and water were provided *ad-libitum*.

Results

The acute median lethal dose (LD_{50}) for the test material was >2 mL/kg for male and female rabbits evaluated in the study. There were no clinical observations and no mortalities during the study.

Conclusions

The acute dermal LD_{50} for the test material was >2 mL/kg.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted as a limit test, with exposure to a single test concentration. The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-1596

Other

Last changed (administrative field for updating): 12/21/04

Primary Skin Irritation

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Not applicable; test substance dose undiluted
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits, 2.3 to 3.0 kg size, were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages.

Skin lesions were evaluated at 24 and 72 hours, and scored in accordance with the methods outlined in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

Following application of 0.5 mL for 24 hours, the test material was determined to be a mild primary skin irritant. No clinical effects or gross mortality observed.

Conclusions

From the results obtained under the experimental conditions employed, a 24-hour application of the test material to the rabbit skin can be designated as a mild primary skin irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-393

Other

Last changed (administrative field for updating): 12/21/04

Primary Skin Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1977
Species/Strain:	New Zealand albino rabbit
Sex:	Male
No. of animals per dose group:	6
Vehicle:	Kerosene
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

Prior to application of the test material in kerosene, the backs of the rabbits were clipped free of hair. The skin was left intact at six test sites and was abraded on the other six. Five-tenths of a milliliter (0.5 mL) of the test material in kerosene was applied to an area of skin approximately 1 in^2 on each rabbit. Patches of surgical gauze measuring 1 in^2, two single layers thick, were applied over the samples and covered with a non-reactive tape. The rabbits were then wrapped with a rubber dam.

After the 24-hour exposure, the dam and tape were removed and the skin reactions evaluated. An evaluation was also made at 72 hours after application.

The reactions were scored according to the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and edema formation score on intact and abraded skin.

Results

Following application of 0.5 mL of test material in kerosene for 24 hours, the test material was determined to be a moderate irritant. It would not be considered a primary skin irritant.

Conclusions

From the results obtained under the experimental conditions employed, a 24-hour application of the test material in kerosene to the rabbit skin can be designated as a moderate irritant. It would not be considered a primary skin irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Huntingdon Life Sciences, Study No. 777-281A

Other

Last changed (administrative field for updating): 12/21/04

Primary Skin Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1977
Species/Strain:	New Zealand albino rabbit
Sex:	Male
No. of animals per dose group:	6
Vehicle:	Aliphatic hydrocarbon
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

Prior to application of the test material in aliphatic hydrocarbon, the backs of the rabbits were clipped free of hair. The skin was left intact at six test sites and was abraded on the other six. Five-tenths of a milliliter (0.5 mL) of the test material in aliphatic hydrocarbon was applied to an area of skin approximately 1 in^2 on each rabbit. Patches of surgical gauze measuring 1 in^2, two single layers thick, were applied over the samples and covered with a non-reactive tape. The rabbits were then wrapped with a rubber dam.

After the 24-hour exposure, the dam and tape were removed and the skin reactions evaluated. An evaluation was also made at 72 hours after application.

The reactions were scored according to the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

Following application of 0.5 mL for 24 hours, the test material in aliphatic hydrocarbon is determined to be a moderate irritant. It would not be considered a primary skin irritant.

Conclusions

From the results obtained under the experimental conditions employed, a 24-hour application of the test material in aliphatic hydrocarbon to the rabbit skin can be designated as a moderate irritant. It would not be considered a primary skin irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Huntingdon Life Sciences, Study No. 777-282A

Other

Last changed (administrative field for updating): 12/21/04

Primary Skin Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbit
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Diluent oil
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits, 2.3 to 3.0 kg size, were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material in diluent oil was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages.

Skin lesions were evaluated at 24 and 72 hours and scored in accordance with the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

Following application of 0.5 mL for 24 hours, the test material in diluent oil is a moderate primary skin irritant. No clinical effects or gross mortality were observed.

Conclusions

From the results obtained under the experimental conditions employed, a 24-hour application of the test material in diluent oil to the rabbit skin can be designated as a moderate primary skin irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-327

Other

Last changed (administrative field for updating): 12/21/04

Primary Skin Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Diluent oil
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits, 2.3 to 3.0 kg, were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material in diluent oil was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages.

Skin lesions were evaluated at 24 and 72 hours, and scored in accordance with the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

Following application of 0.5 mL for 24 hours, the test material in diluent oil was determined to be a moderate primary skin irritant. No clinical effects or gross mortality were observed.

Conclusions

From the results obtained under the experimental conditions employed, a 24-hour application of the test material in diluent oil to the rabbit skin can be designated as a moderate primary skin irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-392

Other

Last changed (administrative field for updating): 12/21/04

Primary Skin Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1980
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Corn oil
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits, 2.3 to 3.0 kg, were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material in corn oil was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 24 hours at which time the patches were removed and the rabbits returned to their cages.

Skin lesions were evaluated at 24 and 72 hours, and scored in accordance with the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

Following application of 0.5 mL for 24 hours, the test material in corn oil was determined to be a mild primary skin irritant. No clinical effects or gross mortality were observed.

Conclusions

From the results obtained under the experimental conditions employed, a 24-hour application of the test material in corn oil to the rabbit skin can be designated as a mild primary skin irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-1312

Other

Last changed (administrative field for updating): 12/21/04

DOT Skin Corrosion

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21, U.S. Department of Transportation (DOT)
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Not applicable; test substance dose undiluted
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 4 hours at which time the patches were removed and the resulting reactions were evaluated for skin corrosion. Following this reading, the test sites were washed to prevent further exposure and the rabbits were returned to their cages.

Skin lesions were evaluated at 24 and 48 hours, and scored in accordance with the methods outlined in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

After exposure for 4 hours, the test material caused no destruction or irreversible alteration to the exposed skin. There was no evidence of corrosion in 48 hours.

Conclusions

The test material is non-corrosive.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-391

Other

Last changed (administrative field for updating): 12/21/04

DOT Skin Corrosion

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21, U.S. Department of Transportation (DOT)
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbit
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Diluent oil
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material in diluent oil was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 4 hours at which time the patches were removed and the resulting reactions were evaluated for skin corrosion. Following this reading, the test sites were washed to prevent further exposure and the rabbits were returned to their cages.

Skin lesions were evaluated at 24 and 48 hours and scored in accordance with the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

After exposure for 4 hours, the test material caused no destruction or irreversible alteration to the exposed skin. No untoward reactions were observed during the study.

Conclusions

Based on the study results, the test material is non-corrosive.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-328

Other

Last changed (administrative field for updating): 12/21/04

DOT Skin Corrosion

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21, U.S. Department of Transportation (DOT)
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Diluent oil
Route of Administration:	Dermal application, occlusive dressing

Remarks Field for Test Conditions

The rabbits were prepared by clipping the skin of the trunk free of hair. Epidermal abrasions were made over a 2 to 3 cm^2 area on each rabbit. Two 2.5 cm^2 gauze patches were placed on each rabbit. One patch was placed over the intact skin, the second patch over the abraded skin. Five-tenths of a milliliter (0.5 mL) of test material in diluent oil was placed under each patch. The patches were secured with tape and covered with a plastic trunk band to prevent evaporation. The rabbits were immobilized in head stocks for 4 hours at which time the patches were removed and the resulting reactions were evaluated for skin corrosion. Following this reading, the test sites were washed to prevent further exposure and the rabbits were returned to their cages.

Skin lesions were evaluated at 24 and 48 hours, and scored in accordance with the methods described in the FHSA. The primary skin irritation of each animal was determined from the sum of the erythema and eschar formation score and the edema formation score on intact and abraded skin.

Results

After exposure for 4 hours, the test material caused no destruction or irreversible alteration to the exposed skin. No evidence of corrosion was seen in 48 hours.

Conclusions

Based on the study results, the test material is non-corrosive.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-390

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Diisononylnaphthalene (CAS No. 63512-64-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Not applicable; test substance dose undiluted
Route of Administration:	Topical

Remarks Field for Test Conditions

One tenth of a milliliter (0.1 mL) of test material was instilled in one eye of each rabbit. The other eye of each rabbit remained untreated and served as a control. The treated eyes were not washed. The rabbits were immobilized in head stocks for 24 hours and then returned to their cages.

Ocular lesions were evaluated at 24, 48, and 72 hours, and at 4, 7, and 14 days. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. The primary eye irritation score for each test group is reflected by the mean of the individual scores of the respective observation time.

Results

Based on the sum of the corneal score, iris score, and conjunctivae score, the test material is a mild eye irritant. There were no untoward reactions during the study.

Conclusions

The undiluted test material is a mild eye irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-396

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid (CAS No. 25322-17-2)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1977
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Aliphatic hydrocarbon
Route of Administration:	Topical

Remarks Field for Test Conditions

One tenth of a milliliter (0.1 mL) of test material in aliphatic hydrocarbon was instilled in one eye of each rabbit. The other eye of each rabbit remained untreated and served as a control. The treated eyes were not washed. The rabbits were immobilized in head stocks for 24 hours and then returned to their cages.

Ocular lesions were evaluated at 24, 48, and 72 hours, and at 4, 7, and 14 days. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. The primary eye irritation score for each test group is reflected by the mean of the individual scores of the respective observation time.

Results

Based on the sum of the corneal score, iris score, and conjunctivae score, the test material is a severe primary eye irritant. There were no untoward reactions during the study.

Conclusions

The test material is a severe primary eye irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-296

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Diluent oil
Route of Administration:	Topical

Remarks Field for Test Conditions

One tenth of a milliliter (0.1 mL) of test material in diluent oil was instilled in one eye of each rabbit. The other eye of each rabbit remained untreated and served as a control. The treated eyes were not washed. The rabbits were immobilized in head stocks for 24 hours and then returned to their cages.

Ocular lesions were evaluated at 24, 48, and 72 hours, and at 4, 7, and 14 days. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. The primary eye irritation score for each test group is reflected by the mean of the individual scores of the respective observation time.

Results

Based on the sum of the corneal score, iris score, and conjunctivae score, the test material is an eye irritant. There were no untoward reactions during the study.

Conclusions

The test material is an eye irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-340

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21, Occupational Safety and Health Administration (OSHA)
GLP (Y/N):	Yes
Year (study performed):	1995
Species/Strain:	New Zealand albino rabbits
Sex:	Male and female
No. of animals per dose group:	3 per sex
Vehicle:	Light mineral oil
Route of Administration:	Topical

Remarks Field for Test Conditions

One-tenth of a milliliter (0.1 mL) of test material in light mineral oil was instilled in the left eye of each rabbit. The eye was gently held shut for approximately 1 second. The other eye of each rabbit remained untreated and served as a control. A plastic Elizabethan collar was placed on each animal after dosing to prevent access to the test site. Both eyes were examined and the test eye scored according to the Draize method at 1, 24, 48, and 72 hours, and at 7 and 10 days after instillation of the test material. All of the test eyes were also examined for the presence of corneal ulcerations at 24 hours with 2% sodium fluorescein. Those eyes with ulcerations were re-stained during each observation period until the ulceration healed.

Clinical observations were recorded at approximately 1- and 4-hours after dosing and daily thereafter, except on the weekend, for the remainder of the study. Body weights were not recorded. All animals were sacrificed by over-exposure to carbon dioxide on Day 10.

Results

Slight corneal opacities and iridial irritation was observed in three of six animals and moderate to severe conjunctival irritation was observed in all animals at 1 hour. Corneal opacities were present in all animals at 24 hours along with corneal ulcerations. The number of corneal ulcerations decreased to three of six animals at 48 hours, and none of the animals at 72 hours. Moderate to severe conjunctival irritation was still present at 24 hours and diminished slowly over the remainder of the study.

Soft stool was noted in all animals on Day 1 and in two of six animals on Day 2. Decreased food consumption and decreased fecal output were noted in two of six animals on Days 2 and 6, respectively. No other clinical observations were noted.

Conclusions

Based on the sum of the corneal score, iris score, and conjunctival score, the test material is an eye irritant.

Data Quality

Reliabilities (Klimisch Code): 1. (Reliable without restrictions)

Remarks Field for Data Reliability

Based on a review of the report, the study was judged to be scientifically defensible.

References

Key Study: Stonybrook Laboratories Inc., Study No. 66245

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1978
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Diluent oil
Route of Administration:	Topical

Remarks Field for Test Conditions

One tenth of a milliliter (0.1 mL) of test material in diluent oil was instilled in one eye of each rabbit. The other eye of each rabbit remained untreated and served as a control. The treated eyes were not washed. The rabbits were immobilized in head stocks for 24 hours and then returned to their cages.

Ocular lesions were evaluated at 24, 48, and 72 hours, and at 4, 7, and 14 days. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. The primary eye irritation score for each test group is reflected by the mean of the individual scores of the respective observation time.

Results

Based on the sum of the corneal score, iris score, and conjunctivae score, the test material is severe eye irritant. There were no untoward reactions during the study.

Conclusions

The test material is a severe eye irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-382

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1980
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	6
Vehicle:	Corn oil
Route of Administration:	Topical

Remarks Field for Test Conditions

One tenth of a milligram (0.1 mg) of test material in diluent oil was instilled in one eye of each rabbit. The eye was gently held shut for approximately 1 second. The other eye of each rabbit remained untreated and served as a control. The treated eyes were not washed. The rabbits were immobilized in head stocks prior to dosing.

Ocular lesions were evaluated at 24, 48, and 72 hours, and at 6, and 7 days. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. The primary eye irritation score for each test group is reflected by the mean of the individual scores of the respective observation time.

Results

Based on the sum of the corneal score, iris score, and conjunctivae score, the test material is minimal eye irritant. There were no untoward reactions during the study.

Conclusions

The test material is a minimal eye irritant.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-1297

Other

Last changed (administrative field for updating): 12/21/04

Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21, Occupational Safety and Health Administration (OSHA)
GLP (Y/N):	Yes
Year (study performed):	1995
Species/Strain:	New Zealand albino rabbits
Sex:	Male and female
No. of animals per sex per dose group:	3 per sex
Vehicle:	Light mineral oil
Route of Administration:	Topical

Remarks Field for Test Conditions

One-tenth of a milliliter (0.1 mL) of test material in light mineral oil was instilled into the left eye of each rabbit. The eye was gently held shut for approximately 1 second. The other eye of each rabbit remained untreated and served as a control. A plastic Elizabethan collar was placed on each animal after dosing to prevent access to the test site. Both eyes were examined and the test eye scored according to the Draize method at 1, 24, 48, and 72 hours, and at 7 and 10 days after instillation of the test material. All of the test eyes were also examined for the presence of corneal ulcerations at 24 hours with 2% sodium fluorescein. Those eyes with ulcerations were re-stained during each observation period until the ulceration healed.

Clinical observations were recorded at approximately 1- and 4-hours after dosing and daily thereafter, except on the weekend, for the remainder of the study. Body weights were not recorded. All animals were sacrificed by over-exposure to carbon dioxide on Day 10.

Results

Slight iridial irritation was observed in two of six animals and moderate to severe conjunctival irritation in all animals at 1 hour. Corneal opacities were present in four of six animals and corneal ulcerations were present in two of six animals at 24 hours. The corneal opacities and ulcerations were no longer

present at 48 hours. Moderate to severe conjunctival irritation was still present at 24 hours and diminished quickly over the remainder of the study.

Soft stool was noted in all animals on Day 1, in three of six animals on Day 2, and in one of six animals on Day 3. Decreased food consumption was observed in two of six animals on Day 1. Decreased fecal output was noted in all animals on Day 6. No other clinical observations were noted.

Conclusions

Based on the sum of the corneal score, iris score, and conjunctival score, the test material is an eye irritant.

Data Quality

Reliabilities (Klimisch Code): 1. (Reliable without restrictions)

Remarks Field for Data Reliability

Based on a review of the report, the study was judged to be scientifically defensible.

References

Key Study: Stonybrook Laboratories Inc., Study No. 66246

Other

Last changed (administrative field for updating): 12/21/04

Modified Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1979
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	12, 4 per group
Vehicle:	Diluent oil
Route of Administration:	Topical

Remarks Field for Test Conditions

The rabbits were subdivided into three groups, with four rabbits evaluated per group. For Group I, one tenth of a milliliter (0.1 mL) of test material in diluent oil was instilled in one eye of each rabbit. For Group II, one tenth of a milliliter (0.1 mL) of test material in diluent oil was instilled in both eyes of each rabbit. The right eye was irrigated with 20 mL of 0.9% saline 10 seconds post-instillation of test material. The left eye was irrigated with 20 mL of U.S.P. mineral oil 10 seconds post-instillation of test material. For Group III, one tenth of a milliliter (0.1 mL) of test material in diluent oil was instilled in both eyes of each rabbit. The right eye was irrigated with 20 mL of U.S.P. mineral oil 10 seconds post-instillation of test material immediately followed with a 20 mL irrigation of 0.9% saline. The left eye was irrigated with 20 mL of U.S.P. mineral oil 30 minutes post-instillation of the test material, immediately followed with a 20 mL irrigation of 0.9% saline.

Ocular lesions were evaluated at 24, 48, and 72 hours, and at 4, 7, and 14 days. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. The primary eye irritation score for each test group is reflected by the mean of the individual scores of the respective observation time. The mean maximum total scores were calculated at 24 and 48 hours, according to the method of Calandra.(Journal of Soc. Cos. Chem.).

Results

The lowest mean maximum total score (MMTS) was observed with saline irrigation alone. This was observed at both 24 and 48 hours after treatment. While mineral oil irrigation reduced irritation relative

to Group I (no irrigation) at 24 hours, it appeared to potentiate the irritation as evidenced by an increased MMTS at 48 hours relative to Group I. The greatest MMTS was observed with mineral oil/saline combinations. The greatest irritation was observed after a 30-minute delay before irrigation with mineral oil/saline. The data suggest that saline or mineral oil irrigation soon after exposure (within 10 seconds) reduces the potential for eye injury.

Conclusions

Saline irrigation as soon as possible after exposure to the test material is the treatment of choice in reducing potential eye injury and/or irritation. While mineral oil irrigation initially reduces irritation within the first 24 hours, it appears to potentiate the irritation post-24 hours.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-677

Other

Last changed (administrative field for updating): 12/21/04

Modified Eye Irritation

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Federal Hazardous Substances Act (FHSA), CFR Title 21
GLP (Y/N):	No
Year (study performed):	1980
Species/Strain:	New Zealand albino rabbits
Sex:	Not defined
No. of animals per dose group:	3
Vehicle:	Diluent oil
Route of Administration:	Topical

Remarks Field for Test Conditions

The study was conducted as an internal research screening modified eye irritation comparison study of test material in diluent oil vs. test material in mineral oil. One tenth of a milliliter (0.1 mL) of test material in diluent oil was instilled in the right eye of each rabbit. One-tenth of a milliliter (0.1 mL) of test material in mineral oil was instilled in the left eye of each rabbit.

Ocular lesions were evaluated at 24, 48, and 72 hours. A primary eye irritation score for each animal was derived from the sum of the corneal score, iris score, and conjunctivae score. After 72 hours, the mean maximum total score (MMTS) score was calculated and irritation classification assigned.

Results

Based on the sum of the corneal score, iris score, and conjunctivae score, the test material diluted in diluent oil is classified as practically non-irritating. The test material diluted in mineral oil is classified as minimally irritating. Observations during the study were not remarkable.

Conclusions

Based on the results of this study, the test material diluted in diluent oil is classified as practically non-irritating. The test material diluted in mineral oil is classified as minimally irritating.

Data Quality

Reliabilities (Klimisch Code): 2. (Reliable with restrictions)

Remarks Field for Data Reliability

The study was conducted prior to adoption of the Good Laboratory Practice (GLP) guidelines.

References

Key Study: Product Safety Labs, Report No. T-769

Other

Last changed (administrative field for updating): 12/21/04

Sensitization

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, calcium salt (CAS No. 57855-77-3

Method

Method/guideline followed:	Human Repeated Insult Patch Test/Sensitization Test
GLP (Y/N):	No
Year (study performed):	1995
Species/Strain:	Human volunteers
Sex:	Not defined
No. of animals per dose group:	104
Vehicle:	Mineral oil
Route of Administration:	Topical

Remarks Field for Test Conditions

The test material was occlusively applied to the skin of the infrascapular area of the back, between the shoulder blades, using Finn Chambers (8 mm inner diameter aluminum chambers affixed to Scanpor tape). The induction phase consisted of nine consecutive occlusive applications of the test material for a period of 3 weeks. The patches were removed approximately 48 hours after each application. The subjects returned to the facility at 48-hour intervals for evaluation of the treated sites, and to have identical patches applied. Following the ninth evaluation, the subjects were released for a 17-day rest period prior to the challenge phase.

The challenge phase was initiated during the sixth week of the study, with identical patches applied to previously unexposed sites. These patches were removed after 48 hours. Skin reactions were graded in a manner identical to that described above.

Results

At challenge, 1 subject out of 104 experienced a reaction suggestive of contact sensitization at the 96-hour observation. A re-challenge test was conducted with this subject in order to determine whether the reaction was due to allergic contact dermatitis. In addition to the test material, the subject was challenged with the test material 10% w/w in mineral oil, test material 5.0% w/w in mineral oil, and the vehicle (100% mineral oil) alone. Upon rechallenge, no reactions indicative of contact sensitization were observed.

Conclusions

Under the conditions employed in this study, the test material did not act as a skin sensitizer under occluded (severe exposure) conditions in any of the 104 human volunteers.

Data Quality

Reliabilities (Klimisch Code): 1. (Reliable without restrictions)

Remarks Field for Data Reliability

Based on a review of the report, the study was judged to be scientifically defensible.

References

Key Study: Stonybrook Laboratory Study No. 66210, Sensitization test conducted by Stephens & Associates, Inc., Study No. C95-0006.

Other

Last changed (administrative field for updating): 12/21/04

Sensitization

Test Substance

Identity: Dinonylnaphthalene sulfonic acid, barium salt (CAS No. 25619-56-1)

Method

Method/guideline followed:	Human Repeated Insult Patch Test/Sensitization Test
GLP (Y/N):	No
Year (study performed):	1995
Species/Strain:	Human volunteers
Sex:	Not defined
No. of animals per dose group:	103
Vehicle:	Mineral oil
Route of Administration:	Topical

Remarks Field for Test Conditions

The test material was occlusively applied to the skin of the infrascapular area of the back, between the shoulder blades, using Finn Chambers (8 mm inner diameter aluminum chambers affixed to Scanpor tape). The induction phase consisted of nine consecutive occlusive applications of the test material for a period of 3 weeks. The patches were removed approximately 48 hours after each application. The subjects returned to the facility at 48-hour intervals for evaluation of the treated sites, and to have identical patches applied. Following the ninth evaluation, the subjects were released for a 17-day rest period prior to the challenge phase.

The challenge phase was initiated during the sixth week of the study, with identical patches applied to previously unexposed sites. These patches were removed after 48 hours. Skin reactions were graded in a manner identical to that described above.

Results

At challenge, 1 subject out of 103 experienced a reaction suggestive of contact sensitization at the 48-hour and 96-hour observations. A re-challenge test was conducted with this subject in order to determine whether the reaction was due to allergic contact dermatitis. In addition to the test material, the subject was challenged with the test material 10% w/w in mineral oil, test material 5.0% w/w in mineral oil, and the vehicle (100% mineral oil) alone. Upon re-challenge, there was one reaction at the

96-hour observation to the test material 10% w/w in mineral oil sample. This reaction was judged to be an irritation response since the other test material concentrations failed to elicit a response.

Conclusions

Under the conditions employed in this study, the test material did not act as a skin sensitizer under occluded (severe exposure) conditions in any of the 103 human volunteers.

Data Quality

Reliabilities (Klimisch Code): 1. (Reliable without restrictions)

Remarks Field for Data Reliability

Based on a review of the report, the study was judged to be scientifically defensible.

References

Key Study: Stonybrook Laboratory Study No. 66209, Sensitization test conducted by Stephens & Associates, Inc., Study No. C95-0001.

Other

Last changed (administrative field for updating): 12/21/04