

AR201-13335B

Neoacids C5-C28 Category

**Robust Summaries
(Environmental Fate and Effects)**

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Prepared by:

ExxonMobil Chemical Company

November 15th, 2001

Robust Summaries - Neoacids C5-C28

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Biodegradation - Manometric Respirometry

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CAS # 26896-20-8; C10 Neo Acid, 2,2-Dimethyl-octanoic acid

Biodegradation -Manometric Respirometry

Invertebrate Acute Toxicity

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CAS # 68938-07-8; C9-13 Neo Acid, Fatty Acids C9-13

Biodegradation -Manometric Respirometry

Robust Summaries - Neoacids C5-C28

Invertebrate Acute Toxicity

Test Substance:	Propanoic acid, 2,2-dimethyl (C5)																													
Method/Guideline:	USEPA -660/3-75-009 Methods for Acute Toxicity with Fish and Macroinvertebrates, and Amphibians, 1975																													
Type (test type):	Daphnid Acute Toxicity Test																													
GLP:	Unknown																													
Year (study performed):	1977																													
Species:	Water Flea (Daphnia magna)																													
Analytical Monitoring:	No																													
Exposure Period:	48 hour																													
Statistical Method:	Moving Average-Angle Method, (Harris 1959)																													
Test Conditions:	<p>For each test concentration, the appropriate amount of test substance was dissolved in ethanol and pipetted into 500ml of dilution water. This solution was mixed with a magnetic stirrer and divided into three 150ml replicates for testing. The remaining 50ml was used for pH and dissolved oxygen measurements. A positive control (with ethanol) and a negative control (dilution water) were also tested. Test vessels were 250ml beakers containing five daphnids each. Dilution water was reconstituted deionized water with a hardness of 180mg/L as CaCO₃, with a pH of 8.0. The test was performed under static conditions with no aeration.</p> <p>Nominal test concentrations were 36, 60, 100, 170, 280, and 460 mg/L</p> <p>Test temperature was 22+/- 1 Deg C. Dissolved oxygen ranged from 8.6 to 8.8 mg/L during the study. The pH of the test solutions varied from Control - 8.3; 36 mg/L - 8.2; 170 mg/L - 7.6; and 460 mg/L - 5.2.</p> <p>Organisms were supplied by in-house cultures. Age = <24 hours old</p>																													
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.																														
Results:	LC50 = 202.94 mg/L (95% CI 241.23 to 168.21) based upon nominal test concentrations.																													
Units/Value:																														
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.																														
	<table><thead><tr><th rowspan="2">Test Concentration</th><th colspan="2">Mean % Mortality</th></tr><tr><th>24 hr.</th><th>48 hr.</th></tr></thead><tbody><tr><td>Positive Control</td><td>0</td><td>0</td></tr><tr><td>Negative Control</td><td>0</td><td>0</td></tr><tr><td>36 mg/L</td><td>0</td><td>0</td></tr><tr><td>60 mg/L</td><td>0</td><td>0</td></tr><tr><td>100 mg/L</td><td>0</td><td>7</td></tr><tr><td>170 mg/L</td><td>7</td><td>13</td></tr><tr><td>280 mg/L</td><td>20</td><td>93</td></tr><tr><td>460 mg/L</td><td>100</td><td>100</td></tr></tbody></table>	Test Concentration	Mean % Mortality		24 hr.	48 hr.	Positive Control	0	0	Negative Control	0	0	36 mg/L	0	0	60 mg/L	0	0	100 mg/L	0	7	170 mg/L	7	13	280 mg/L	20	93	460 mg/L	100	100
Test Concentration	Mean % Mortality																													
	24 hr.	48 hr.																												
Positive Control	0	0																												
Negative Control	0	0																												
36 mg/L	0	0																												
60 mg/L	0	0																												
100 mg/L	0	7																												
170 mg/L	7	13																												
280 mg/L	20	93																												
460 mg/L	100	100																												
Conclusion:	Test substance is considered to be of low toxicity																													
Reliability:	Code 2, Reliable with Restriction																													

Robust Summaries - Neoacids C5-C28

Lack of analytical verification, concentration of ethanol unknown, missing pH value of 280mg/L concentration, quality assurance unknown.

Reference:

EG&G Bionomics, Wareham, Mass.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	Propanoic acid, 2,2-dimethyl (C5)
Method/Guideline:	Standard Methods for the Examination of Water and Wastewater Method #231, 1971
Type (test type):	Fish Static Acute Toxicity Test
GLP:	No
Year (study performed):	1979
Species:	Gold Fish (<i>Crassius auratus</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Interpolation of graph of log of concentration (APHA 1971)
Test Conditions:	<p>The test material was added to ~30 L glass tank containing laboratory dilution water. Each chemical was tested in a series of concentrations in 25 L of solution. All tanks contained 10 fish. All test solutions were aerated unless it was a volatile compound.</p> <p>Test temperature was 20 +/- 1 Deg C., Lighting was not reported Dissolved Oxygen = test solutions aerated during study. The pH was 5.4.</p> <p>Fish Mean Wt.= 3.3 +/- 1.0g. Mean Total length = 6.2 +/-cm, Test Loading = 1.3 g of fish/L.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	
Results:	
Units/Value:	LC50 = 380mg/L
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was Total Organic Carbon or by extraction and subsequent GC analysis.
Conclusion:	Test substance is considered to have low toxicity
Reliability:	Code 2, Reliable with Restriction
	Minimal data presented (i.e. lacking conc. series, analytical measurements, Dissolved Oxygen measurements).
Reference:	Bridie, A.L. et al., The Acute Toxicity Test of some Petrochemicals to Goldfish. Water Research Vol. 13. 1979
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Neoacids C5-C28

Biodegradation

Test Substance:	Propanoic acid 2,2-dimethyl (C5)									
Method/Guideline:	OECD 301F, 1992									
Type (test type):	Manometric Respirometry Test									
GLP:	Yes									
Year (study performed):	1996									
Inoculum:	Domestic activated sludge									
Exposure Period:	28 days									
Test Conditions:	<p>Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was between 31 and 50 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/- 1 Deg C.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p>									
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.										
Results:										
Units/Value:	<p>Test material was not readily biodegradable. Half-life was not reached. By day 28, 24% degradation of the test material was observed. 10% biodegradation was achieved on day 20. By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.</p>									
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.										
	<table><thead><tr><th></th><th>% Degradation* (day 28)</th><th>Mean % Degradation (day 28)</th></tr></thead><tbody><tr><td>Test Material</td><td>18.9, 42.7, 10.7</td><td>24.1</td></tr><tr><td>Na Benzoate</td><td>98.9, 95.5</td><td>97.2</td></tr></tbody></table>		% Degradation* (day 28)	Mean % Degradation (day 28)	Test Material	18.9, 42.7, 10.7	24.1	Na Benzoate	98.9, 95.5	97.2
	% Degradation* (day 28)	Mean % Degradation (day 28)								
Test Material	18.9, 42.7, 10.7	24.1								
Na Benzoate	98.9, 95.5	97.2								
	* replicate data									
Conclusion:	Test substance is considered not readily biodegradable.									
Reliability:	Code 1, Reliable without Restrictions									
Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 136894A..									
Other (source):	ExxonMobil Biomedical Sciences, Inc.									

Robust Summaries - Neoacids C5-C28

Biodegradation

Test Substance:	Carboxylic acid, C6-8 neo												
Method/Guideline:	OECD 301F, 1992												
Type (test type):	Manometric Respirometry Test												
GLP:	Yes												
Year (study performed):	1996												
Inoculum:	Domestic activated sludge												
Exposure Period:	28 days												
Test Conditions:	<p>Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was between 31 and 50 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/- 1 Deg C.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p>												
Results:													
Units/Value:	<p>Test material was not readily biodegradable. Half-life was not reached. By day 28, 44% degradation of the test material was observed. 10% biodegradation was achieved on day 19. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.</p>												
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.													
	<table><thead><tr><th></th><th>% Degradation*</th><th>Mean % Degradation</th></tr><tr><th><u>Sample</u></th><th><u>(day 28)</u></th><th><u>(day 28)</u></th></tr></thead><tbody><tr><td>Test Material</td><td>62.8, 24.6, 44.6</td><td>44.0</td></tr><tr><td>Na Benzoate</td><td>98.9, 95.5</td><td>97.2</td></tr></tbody></table>		% Degradation*	Mean % Degradation	<u>Sample</u>	<u>(day 28)</u>	<u>(day 28)</u>	Test Material	62.8, 24.6, 44.6	44.0	Na Benzoate	98.9, 95.5	97.2
	% Degradation*	Mean % Degradation											
<u>Sample</u>	<u>(day 28)</u>	<u>(day 28)</u>											
Test Material	62.8, 24.6, 44.6	44.0											
Na Benzoate	98.9, 95.5	97.2											
	* replicate data												
Conclusion:	Test substance is considered not readily biodegradable.												
Reliability:	Code 1, Reliable without Restrictions												
Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 136894A..												
Other (source):	ExxonMobil Biomedical Sciences, Inc.												

Fish Acute Toxicity

Test Substance: Carboxylic acid, C6-8 neo

Method/Guideline: US EPA TSCA 797.1400

Type (test type): Fish Acute Flow-through Toxicity Test

GLP: Yes

Year (study performed): 1993

Species: Fathead Minnow (*Pimephales promelas*)

Analytical Monitoring: Yes

Exposure Period: 96 hour

Statistical Method: Graphical (EPA-600/4-90-027)

Test Conditions: A stock solution of 900mg/L was prepared daily and administered via a stainless steel and glass proportional diluter to achieve the desired study concentrations. The stock solution was mixed for 30 minutes and adjusted to a pH of 7.5 +/- 0.1 as needed. All test material went into solution. The test chambers were duplicate 1L glass dishes located within 19L glass aquaria with a flow rate of 6 dish volumes per day. Each dish contained 10 fish.

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Test temperature was 22.8 Deg C., Lighting was 16 hours light : 8 hours dark with 51.8 to 52.9 ft-candles during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 8.5 mg/L and from 6.6 to 8.0 mg/L at termination. The pH was ranged from 7.6 to 7.2 during the study.

Fish Mean Wt.= 0.065g. Mean Total length = 1.6cm, Test Loading = 0.11 g of fish/L.

Results:

LC50 = 630mg/L, based upon measured concentrations.

Units/Value:

Analytical method used was GC-FID

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.</u>
Control	<0.79 mg/L	0
56.25 mg/L	51.4 mg/L	0
112.5 mg/L	124 mg/L	0
225 mg/L	200 mg/L	0
450 mg/L	436 mg/L	0
900 mg/L	882 mg/L	0

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Conclusion:	Test substance is considered low toxicity
Reliability:	Code 1, Reliable without Restrictions
Reference:	Exxon Biomedical Sciences, Inc. Fish Acute Flow-through Toxicity Test, 148641.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Neoacids C5-C28

Algal Toxicity

Test Substance:	Carboxylic acid, C6-8 neo
Method/Guideline:	US EPA TSCA 40 CFR792.1989
Type (test type):	Algal Toxicity Test
GLP:	Yes
Year (study performed):	1993
Species/Strain:	Fresh water Green Algae (Selenastrum capricornutum)
Analytical Monitoring:	Yes
Exposure Period:	72 hour
Statistical Method:	Linear Interpolation

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organism culture, age.**

A 500mg/L stock solution was prepared by adding the appropriate amount of test substance to algal nutrient media in an aspirator bottle. The stock solution was mixed for 15 minutes at <10% vortex on a magnetic stir plate. After mixing the solution was drawn out the bottom port. The pH was adjusted to 7.5 +/- 0.1 as necessary. The stock was diluted with algal nutrient media to prepared test solutions. Three replicates and a media/toxicant blank were prepared for each concentration. Replicate vessels were 125ml autoclaved Erlenmeyer flasks sealed with gauze stoppers. Test flasks (except blanks) were inoculated with ~1.0E⁴ cells/ml of algae. All test vessels were placed on a shaker table at ~100 rpm during the study.

Nominal treatment levels were 8.0, 31.0, 62, 125, and 250mg/L

Test temperature was 23.9 Deg. C. Lighting was continuous at 399.8 to 411.65 ft candles. The pH was 7.5 at test initiation and ranged from 7.4 to 7.6 at test termination.

Results:

96 hour EC50 = 6.49mg/L (95% CI 5.64 to 7.54) based upon initial measured values (day 0).

Units/Value:

Measurement (cells/growth)

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Nominal Conc.</u> (mg/L)	<u>Measured Conc.</u> Day 0 (mg/L)	<u>Mean Cells</u> at 96 hr	<u>% Inhibition</u> at 96 hr
Control	0	2.3 E6	-
3.12	3.03	2.3 E6	0
6.25	6.20	1.2 E6	47.8
12.5	12.24	4.8 E5	79.1
25.0	23.55	4.2 E5	81.7
50.0	52.15	3.6 E5	84.3

Conclusion:

Test substance is considered moderately toxic

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Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences Inc., Algal Acute Toxicity Test, 148667

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Neoacids C5-C28

Biodegradation

Test Substance:	2,2-Dimethyloctanoic Acid (C10)									
Method/Guideline:	OECD 301F, 1992									
Type (test type):	Manometric Respirometry Test									
GLP:	Yes									
Year (study performed):	1996									
Inoculum:	Domestic activated sludge									
Exposure Period:	28 days									
Test Conditions:	<p>Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was between 31 and 50 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/- 1 Deg C.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p>									
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.										
Results:										
Units/Value:	<p>Test material was not readily biodegradable. Half-life was not reached. By day 28, 11% degradation of the test material was observed. 10% biodegradation was achieved on day 27</p> <p>By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.</p> <p>Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.</p>									
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.										
	<table><thead><tr><th><u>Sample</u></th><th><u>% Degradation* (day 28)</u></th><th><u>Mean % Degradation (day 28)</u></th></tr></thead><tbody><tr><td>Test Material</td><td>20.5, 3.60, 8.90</td><td>11.0</td></tr><tr><td>Na Benzoate</td><td>98.9, 95.5</td><td>97.2</td></tr></tbody></table>	<u>Sample</u>	<u>% Degradation* (day 28)</u>	<u>Mean % Degradation (day 28)</u>	Test Material	20.5, 3.60, 8.90	11.0	Na Benzoate	98.9, 95.5	97.2
<u>Sample</u>	<u>% Degradation* (day 28)</u>	<u>Mean % Degradation (day 28)</u>								
Test Material	20.5, 3.60, 8.90	11.0								
Na Benzoate	98.9, 95.5	97.2								
	* replicate data									
Conclusion:	Test substance is considered not readily biodegradable.									
Reliability:	Code 1, Reliable without Restrictions									
Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 136894A..									
Other (source):	ExxonMobil Biomedical Sciences, Inc.									

Robust Summaries - Neoacids C5-C28

Invertebrate Acute Toxicity

Test Substance:	2,2-Dimethyloctanoic Acid (C10)																																
Method/Guideline:	USEPA -660/3-75-009 Methods for Acute Toxicity with Fish and Macroinvertebrates, and Amphibians, 1975																																
Type (test type):	Daphnid Acute Toxicity Test																																
GLP:	No																																
Year (study performed):	1977																																
Species:	Water Flea (Daphnia magna)																																
Analytical Monitoring:	No																																
Exposure Period:	48 hour																																
Statistical Method:	Moving Average-Angle Method, (Harris 1959)																																
Test Conditions:	<p>For each test concentration, the appropriate amount of test substance was dissolved in triethylene glycol (TEG) and pipetted into 500ml of dilution water. This solution was mixed with a magnetic stirrer and divided into three 150ml replicates for testing. The remaining 50ml was used for pH and dissolved oxygen measurements. A positive control (with TEG) and a negative control (dilution water) were also tested. Test vessels were 250ml beakers containing five daphnids each. Dilution water was reconstituted deionized well water with a hardness of 180mg/L as CaCO₃, with a pH of 8.0. The test was performed under static conditions with no aeration.</p> <p>Nominal test concentrations were 13, 22, 36, 60, 100, 170, and 280 mg/L</p> <p>Test temperature was 22+/- 1 Deg C. Dissolved oxygen ranged from 8.6 to 8.8 mg/L during the study. The pH of the test solutions ranged from 7.1 to 8.2.</p> <p>Organisms were <24 hrs old, supplied by in-house cultures</p>																																
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.																																	
Results:	LL50 = 47.1 mg/L (95% CI 33.6 to 57.8) based upon nominal test concentrations.																																
Units/Value:																																	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	<table><thead><tr><th rowspan="2"><u>Test Concentration</u></th><th colspan="2"><u>Mean % Mortality</u></th></tr><tr><th><u>24 hr.</u></th><th><u>48 hr.</u></th></tr></thead><tbody><tr><td>Positive Control</td><td>0</td><td>0</td></tr><tr><td>Negative Control</td><td>0</td><td>0</td></tr><tr><td>13 mg/L</td><td>0</td><td>13</td></tr><tr><td>22 mg/L</td><td>0</td><td>13</td></tr><tr><td>36 mg/L</td><td>0</td><td>20</td></tr><tr><td>60 mg/L</td><td>20</td><td>67</td></tr><tr><td>100 mg/L</td><td>53</td><td>100</td></tr><tr><td>170 mg/L</td><td>87</td><td>100</td></tr><tr><td>280 mg/L</td><td>73</td><td>100</td></tr></tbody></table>	<u>Test Concentration</u>	<u>Mean % Mortality</u>		<u>24 hr.</u>	<u>48 hr.</u>	Positive Control	0	0	Negative Control	0	0	13 mg/L	0	13	22 mg/L	0	13	36 mg/L	0	20	60 mg/L	20	67	100 mg/L	53	100	170 mg/L	87	100	280 mg/L	73	100
<u>Test Concentration</u>	<u>Mean % Mortality</u>																																
	<u>24 hr.</u>	<u>48 hr.</u>																															
Positive Control	0	0																															
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60 mg/L	20	67																															
100 mg/L	53	100																															
170 mg/L	87	100																															
280 mg/L	73	100																															
Conclusion:	Test substance is considered to be of moderate toxicity																																

Robust Summaries - Neoacids C5-C28

Reliability: Code 2, Reliable with Restrictions
Lack of measured concentrations, no documentation of pH adjustment of treatments.

Reference: EG&G Bionomics, Wareham, Mass. BW-78-1-005

Other (source): ExxonMobil Biomedical Sciences, Inc.

Fish Acute Toxicity

Test Substance:	2,2-Dimethyloctanoic Acid (C10)
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1996
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Bionomial Method
Test Conditions:	<p>Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solution was mixed for 24 hours at a vortex of $\leq 10\%$ of the total depth. After mixing the mixtures were adjust for pH to that of the dilution water using 1.0m NaOH. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing $\sim 80\%$ of the test solution through the port at the bottom and refilling with fresh solution.</p> <p>Test temperature was 15.0 Deg C., Lighting was 19 hours light : 5 hours dark with 528 to 538 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.5 to 9.0 mg/L and from 5.9 to 7.4 mg/L in "old" solutions prior to renewals. The pH was ranged from 7.0 to 7.6 during the study. Fish were not fed during the study.</p> <p>Fish Mean Wt. = 0.260g. Mean Total length = 3.3cm, Test Loading = 0.29 g of fish/L.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	
Results:	
Units/Value:	LC50 = 37.2mg/L (CI 26.3 to 52.5), based upon measured concentrations of mean of old and new samples.
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was GC-FID LL50 = 35.4 mg/L (CI 25.0 to 50.0), based upon nominal loading levels.

Robust Summaries - Neoacids C5-C28

Results continued	<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.</u>
	Control	Below detection	0
	6.25 mg/L	10.3 mg/L	0
	12.5 mg/L	13.6 mg/L	0
	25 mg/L	26.3 mg/L	0
	50 mg/L	52.5 mg/L	100
	100 mg/L	102 mg/L	100

Conclusion:

Test substance is considered moderate toxicity

Reliability:

Code 1, Reliable without Restrictions

Reference:

Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118358.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Neoacids C5-C28

Biodegradation

Test Substance:	Fatty Acids C9-13, Neo 913 Acid									
Method/Guideline:	OECD 301F, 1992									
Type (test type):	Manometric Respirometry Test									
GLP:	Yes									
Year (study performed):	1996									
Inoculum:	Domestic activated sludge									
Exposure Period:	28 days									
Test Conditions:	<p>Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was between 31 and 50 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/- 1 Deg C.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p>									
Results:										
Units/Value:	<p>Test material was not readily biodegradable. Half-life was not reached. By day 28, 2.3% degradation of the test material was observed. 10% biodegradation was not achieved by day 28. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.</p>									
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.										
	<table><thead><tr><th>Sample</th><th>% Degradation* (day 28)</th><th>Mean % Degradation (day 28)</th></tr></thead><tbody><tr><td>Test Material</td><td>4.50, 0.00, 2.50</td><td>2.33</td></tr><tr><td>Na Benzoate</td><td>98.9, 95.5</td><td>97.2</td></tr></tbody></table>	Sample	% Degradation* (day 28)	Mean % Degradation (day 28)	Test Material	4.50, 0.00, 2.50	2.33	Na Benzoate	98.9, 95.5	97.2
Sample	% Degradation* (day 28)	Mean % Degradation (day 28)								
Test Material	4.50, 0.00, 2.50	2.33								
Na Benzoate	98.9, 95.5	97.2								
	* replicate data									
Conclusion:	Test substance is considered not readily biodegradable.									
Reliability:	Code 1, Reliable without Restrictions									
Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 136894A..									
Other (source):	ExxonMobil Biomedical Sciences, Inc.									

Robust Summaries - Neoacids C5-C28

Neoacids (C₅-C₂₈) Category

Robust Summaries (Mammalian Toxicity)

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Prepared by:

ExxonMobil Chemical Company

November 15, 2001

Table of Contents

CAS # 75-98-9; Propanoic acid, 2,2-dimethyl-

Acute Oral
Acute Dermal
Acute Inhalation
Repeat Dose - Dermal

CAS # 95823-36-2; Carboxylic acid, C6-8 neo

Acute Oral
Acute Dermal
Acute Inhalation
Repeat Dose - Dermal
Developmental Toxicity

CAS #26896-20-8; 2,2-Dimethyloctanoic acid

Acute Oral
Acute Dermal
Acute Inhalation (vapor)
Acute Inhalation (aerosol)
Repeat Dose - Dermal
Reproductive Toxicity

CAS # 25103-52-0; Isooctanoic acid (read-across)

Developmental Toxicity
Reproductive Toxicity

CAS #3302-10-1; Isononanoic acid (read-across)

Reproductive Toxicity

Robust Summaries - Neocids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Propanoic acid, 2,2-dimethyl- 75-98-9</p> <p>Other Acute oral toxicity Pre-GLP 1964 Sprague-Dawley Rats Males 5/dose Gastric Intubation None Single Dose 34.6, 120, 417, 1450, 5000, and 10000 mg/kg None</p> <p>The animals were fasted for a period of three to four hours prior to treatment. The animals were observed for toxic effects and mortality at one, four and 24 hours; and once daily thereafter for 14 days. A necropsy was performed on any animal that died. All surviving animals were weighed, sacrificed and necropsied.</p> <p>LD₅₀= 2000 mg/kg Number of animals dead per number tested: 34.6, 120 and 417 mg/kg: 0/5 1450 mg/kg: 2/5 5000 mg/kg: 5/5 10,000 mg/kg: 5/5</p> <p>There were no deaths and no findings at necropsy in animals treated with 34.6, 120 and 417 mg/kg. At the 1450 mg/kg level, 2 of 5 animals died by day 2 and the remaining animals survived until the end of the study. These animals showed depression, severe dyspnea, depressed reflexes, sprawling, and lack of coordination. All animals in the 5000 and 10,000 mg/kg dose groups died within 48 hours of treatment. Severe depression, dyspnea, and prostration preceded death in all of the animals that died. Necropsy findings in high dose animals indicated congestion of lungs, liver, kidneys, and adrenals.</p> <p>Under conditions of this study, Propanoic acid, 2,2-dimethyl- acid has a low order of acute oral toxicity in rats.</p> <p>2 - Valid with restrictions (Pre-GLP)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>October, 2000</p>
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Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Propanoic acid, 2,2-dimethyl- 75-98-9</p> <p>Other Acute dermal toxicity Pre-GLP 1964 Rabbits/Albino Males and Females 2/sex/dose Dermal None Single Dose 50, 200, 794, 3160 mg/kg None</p> <p>Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.</p> <p>LD50 = 3160 mg/kg</p> <p>In the highest dose group, two deaths occurred at 24 and 48 hours after exposure to the test substance. Death was preceded by marked depression, severe, dyspnea, prostration, excessive urination, and coma. Necropsy revealed congestion of the lungs, adrenals, kidneys, and blanched areas on the liver and spleen. In addition, inflammation of the bladder and gastrointestinal tract were noted. In the 794 mg/kg group, three of the four animals exhibited slight depression, dyspnea, unsteady gait with slight sprawling of the limbs at 24 hours after exposure to the test substance. However, by the third day post-exposure, all of the animals appeared normal. At the termination of the study, necrotic tissue was seen in the abdominal skin at the site of application of the test substance. Otherwise, no gross pathology was observed. In animals exposed to 50 and 200 mg/kg of the test substance, no signs of systemic toxicity were observed. These animals exhibited normal weight gain, appearance, and behavior.</p> <p>Dermal irritation was noted at all dose levels and was characterized by slight, transient erythema, edema, atonia, and desquamation at the lowest level. There was a dose-dependent increase in the intensity and persistence with pronounced irritation at the highest dose levels characterized by blanching, eschar formation, and necrosis.</p> <p>Under conditions of this study, Propanoic acid, 2,2-dimethyl- has a low order of acute dermal toxicity in rabbits.</p> <p>2 - Valid with restrictions (Pre-GLP)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>January, 2001</p>
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Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Propanoic acid, 2,2-dimethyl- 75-98-9</p> <p>Other Acute inhalation toxicity Pre-GLP 1964 Rats Wistar, Mice/Swiss albino Males 10/species Inhalation Other Single 6-hour exposure Saturated vapors - the mean nominal concentration was 4.0 mg/L. A group of mice and rats that served as a common control for the substances tested in this study were sacrificed and examined grossly.</p> <p>An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 29 ml of liquid was vaporized at a flow rate of 23 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were necropsied.</p> <p>Mouse LC50 < 4.0 mg/L Rat > 4.0 mg/L</p> <p>No deaths occurred among any of the animals during the inhalation exposure. Hyperactivity followed by prostration was observed in mice. All 10 mice died within the 24 hours following exposure. Two rats died on the second and fifth days. Rats displayed piloerection, epistaxis, and dyspnea following exposure. Due to advanced autolysis, necropsy of the animals that died did not reveal any meaningful findings. Necropsy of the animals that survived until termination of the study did not reveal any significant gross pathology.</p> <p>Propanoic acid, 2,2-dimethyl- has a moderate order of inhalation toxicity in rodents.</p> <p>2 - Valid with restrictions - No vapor concentration verification (analytical)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>January, 2001</p>
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Robust Summaries - Neoacids C5-C28

Repeat Dose Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Statistical method</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p>	<p>Propanoic acid, 2,2-dimethyl- 75-98-9</p> <p>Other Repeat dermal application Pre-GLP 1964 Albino Rabbits Male 4/dose Dermal Isopropyl Alcohol (IPA) 10 applications with a two-day rest between the 5th and 6th applications. 30mg/kg and 300mg/kg weight/volume solution in isopropyl alcohol Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. Not reported</p> <p>The test material was applied to clipped abdominal skin. A loose gauze binder or a collar was used to prevent ingestion of the test substance. Animals were housed individually and allowed free access to food and water. Each animal was weighed, sacrificed, and necropsied 24 hours after the final application of test material. At the beginning of the study and prior to the final application, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on sections of liver and kidney. Sections of brain, thyroid, lungs, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis.</p> <p>For systemic effects: NOAEL = 300 mg/kg Propanoic acid, 2,2-dimethyl- produced moderate to severe skin irritation.</p> <p>The control animals exhibited normal appearance and behavior throughout the study with the exception of nasal discharge in one animal and diarrhea in another. Slight body weight loss was observed during the first week, but the animals regained the weight and most animals showed overall weight gains by the end of the study. No treatment-related effects were observed at gross necropsy. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits.</p> <p>Control animals exhibited slight erythema throughout the study and slight atonia and desquamation following the fifth application. Animals that received the test substance exhibited normal appearance and behavior throughout the study. Animals in the low dose group showed a net body weight gain by the end of the study and animals in the high dose group showed a slight weight loss by the end of the study. Gross pathological findings revealed parasitic infection of the liver and pitted kidneys in one rabbit, congested lungs in another, and congestion in the pancreas and kidney of a third rabbit. Slight to moderate erythema was observed in the low dose animals. Animals in the high dose group displayed moderate erythema, moderate edema, and moderate to marked atonia and desquamation. Three of the animals in the high dose group had areas of necrosis that persisted through the study.</p>
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Robust Summaries - Neoacids C5-C28

Conclusions	Under the conditions of this study, Propanoic acid, 2,2-dimethyl- has a low order of systemic toxicity following repeated dermal exposure.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Hazleton Laboratories, Inc. (1964) "Repeated Dermal Application - Rabbits," Unpublished report.
Date last changed	January 2001

Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Carboxylic acid, C6-8 neo 95823-36-2</p> <p>Other Acute oral toxicity Pre-GLP 1964 Sprague-Dawley Rats Males 5/dose Gastric Intubation None Single Dose 34.6, 120, 417, 1450, 5000, and 10000 mg/kg None</p> <p>The animals were fasted for a period of three to four hours prior to treatment. The animals were observed for toxic effects and mortality at one, four and 24 hours; and once daily thereafter for 14 days. Necropsy was performed on any animal that died. All surviving animals were weighed, sacrificed and necropsied.</p> <p>LD₅₀= 1860 mg/kg</p> <p>There were no principal toxic effects at 34.6, 120 and 417 mg/kg. In addition there were no findings at necropsy in these animals. At 1450 mg/kg, although there were no findings at necropsy, clinical signs were observed after dosing which included depression, dyspnea and slight to marked ataxia. At the two highest dose levels, all animals were dead within 24 hours. Prior to death, animals exhibited marked depression, sprawling of the limbs and depressed reflexes. Congestion of the lungs, kidneys and adrenals were observed in these animals.</p> <p>Under conditions of this study, Carboxylic acid, C6-8 neo acid has a low order of acute oral toxicity in rats.</p> <p>2 - Valid with restrictions (Pre-GLP)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>January, 2001</p>
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Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Carboxylic acid, C6-8 neo 95823-36-2</p> <p>Other Acute dermal toxicity Pre-GLP 1964 Albino Rabbits Males and Females 2/sex/dose Dermal None Single Dose 50, 200, 794, 3160 mg/kg None</p> <p>Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.</p> <p>LD50 > 3160 mg/kg</p> <p>One death occurred in the 200 mg/kg group at 48 hours post-exposure, but this was not considered to be treatment-related, since no deaths occurred in any of the other treatment groups. Upon necropsy, cecal obstruction and a large amount of fluid in the abdominal cavity were found. No signs of systemic toxicity were seen in any of the animals exposed to 50, 200, or 794 mg/kg. In the highest dose group, marked depression, dyspnea, ataxia, and sprawling of the limbs were observed 1 to 4 hours after application. However, the animals had completely recovered by 24 hours following exposure and exhibited normal appearance and behavior for the remainder of the 14-day post-exposure period. Necropsy revealed no significant signs of gross pathology in these animals.</p> <p>Dose-dependent dermal irritation occurred at all of the doses tested. This ranged from slight to moderate erythema, atonia, and desquamation at the lower dose levels to moderate erythema and edema with atonia and desquamation at the two higher dose levels.</p> <p>Under conditions of this study, Carboxylic acid, C6-8 neo acid has a low order of acute dermal toxicity in rabbits.</p> <p>2 - Valid with restrictions (Pre-GLP)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>January, 2001</p>
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Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Carboxylic acid, C6-8 neo 95823-36-2</p> <p>NA Acute inhalation toxicity Pre-GLP 1964 Rats/Albino, Mice/Albino Males 10/species Inhalation None Single 6-hour exposure Saturated vapors - the mean nominal concentration was 3.0 mg/L. Groups of mice and rats that served as common controls for the substances tested in this study were sacrificed and examined grossly.</p> <p>An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 31 ml of liquid was vaporized at a flow rate of 27 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were necropsied.</p> <p>LD50 > 3.0 mg/L</p> <p>No significant toxic signs were observed during the 6-hour exposure period. All mice and rats appeared normal up to 5 days following exposure, when the mice developed urticaria. No deaths occurred in mice or rats throughout the study and no significant observations were made at necropsy.</p> <p>Under conditions of this study, Carboxylic acid, C6-8 neo has a low order of acute inhalation toxicity in mice and rats.</p> <p>2 - Valid with restrictions - No vapor concentration verification (analytical)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>January, 2001</p>
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Robust Summaries - Neoacids C5-C28

Repeat Dose Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Statistical method</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p>	<p>Carboxylic acid, C6-8 neo 95823-36-2</p> <p>Other Repeat dermal application Pre-GLP 1964 Albino Rabbits Male 4/dose Dermal None 10 applications with a two-day rest between the 5th and 6th applications. 55.4 mg/kg, 553.7 mg/kg Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. Not reported</p> <p>The test material was applied to clipped abdominal skin. A loose gauze binder or a collar was used to prevent ingestion of the test substance. Animals were housed individually and allowed free access to food and water. Each animal was weighed, sacrificed, and necropsied 24 hours after the final application of test material. At the beginning of the study and prior to the final application, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on sections of liver and kidney. Sections of brain, thyroid, lungs, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis.</p> <p>For systemic effects: NOAEL = 553.7 mg/kg Carboxylic acid, C6-8 neo produced moderate to severe skin irritation.</p> <p>Animals in the low dose group showed normal appearance behavior throughout the study. With the exception of one animal that showed a slight weight loss, the animals in the low dose group showed an overall body weight gain. In the high dose group, 3 of the 4 animals displayed normal appearance and behavior and either maintained their weight or had a slight weight loss. From the fifth through the ninth application, the fourth animal had labored breathing, weight loss, and was found dead 24 hours after the final application. Upon necropsy, this animal had congested and emphysematous lungs in addition to hemorrhagic areas in the renal medulla. The death of this animal was deemed to be unrelated to the treatment. Gross pathology of the remaining animals of the high dose group did not reveal any abnormalities other than a slight parasitic infection in the liver of one of the rabbits. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits.</p> <p>In the low dose animals, slight erythema was observed during the first week, with slight to moderate atonia and desquamation that followed the third application and lasted through the study. At the highest dose, slight to moderate erythema was observed and slight to moderate edema was present from the second through the fifth applications. After the fourth application, moderate to marked atonia, desquamation, and slight fissuring was observed through the remainder of the study. All animals showed areas of necrosis at the application site and in two animals, the skin was hypersensitive to touch.</p>
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Robust Summaries - Neoacids C5-C28

Conclusions	Under the conditions of this study, Carboxylic acid, C6-8 neo has a low order or systemic toxicity following repeated dermal exposure.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Hazleton Laboratories, Inc. (1964) "Repeated Dermal Application - Rabbits," Unpublished report.
Date last changed	January 2001

Robust Summaries - Neoacids C5-C28

Developmental Toxicity

<p>Test Substance CAS No.</p> <p>Method Type of Study GLP Year Species/Strain Sex Number/sex/dose Route of administration Exposure Period Concentrations Controls Statistical methods</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks for Results</p>	<p>Carboxylic acid, C6-8 neo 95823-36-2</p> <p>OECD 414 Developmental toxicity Yes 1986 Sprague-Dawley Rats Pregnant Females 22/dose Oral gavage Days 6-15 of gestation 0, 50, 250, 600, or 800 mg/kg Controls received 800 mg/kg of distilled water ANOVA, Kruskal-Wallis, Fisher's exact test</p> <p>Physical examinations were performed and body weight and food consumption were measured throughout gestation. Mated females were sacrificed on gestational day 20 and a gross necropsy was performed. Uteri and ovaries were weighed and corpora lutea were counted. The number of implantation sites, early and late resorptions, and live and dead fetuses were determined. Full term fetuses were examined for abnormalities, weight, and crown-rump distance. From each litter, the heads of half of the fetuses were preserved and examined, while the other half of the fetuses were examined for skeletal malformations and ossification variations.</p> <p>NOAEL fetal: 250 mg/kg NOAEL maternal: 250 mg/kg</p> <p>Maternal: The high dose of 800 mg/kg produced morbidity and mortality in 4 of the 22 mated females. This group displayed lethargy, abnormal breathing, rales, and staining around the muzzle and anogenital areas. Animals in the 600 mg/kg group had a significant incidence of rales. In the high dose group (800 mg/kg), maternal body weight gain and uterine weight at term were significantly reduced. In the 600 mg/kg group, there was a significant reduction in body weight gain during the intervals of gd6-9 and gd0-20. Maternal food consumption was significantly reduced during gestational intervals gd6-9 and gd9-12 for both the 600 and 800 mg/kg groups and during gd12-16 in the 800 mg/kg group.</p> <p>Fetus: In the high dose group, there was a significant increase in early embryonic resorptions with a corresponding decrease in the mean number of live fetuses. The remaining fetuses in the high dose group had significantly reduced fetal body weight and crown-rump distance. Microphthalmia and anophthalmia were observed in 14% of the fetuses from the high dose group. In addition, fused cervical vertebrae and misaligned thoracic vertebra were observed in the high dose group. Significant incidences of hydrocephalus and structural malformation of thoracic ribs occurred in both the 600 and 800 mg/kg groups. The fraction of malformed fetuses/live fetuses was significantly increased in the 600 and 800 mg/kg groups. In the 250 mg/kg group, there was an increase in the fraction of implants affected, however, this was not significantly different from the control group.</p>
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Robust Summaries - Neoacids C5-C28

Results, continued	<p>Visceral examination revealed that the incidence of renal/ureter variations was significantly increased in the high dose group. In addition, the high dose group showed an increased incidence of unossified structures of the cranium, sternum, vertebrae, pelvis, and hindpaw. In both the 600 and 800 mg/kg groups, there were increases in the incidences of incompletely ossified supraoccipital and cervical vertebrae.</p>
Conclusions	<p>Carboxylic acid, C6-8 neo is embryo-lethal and teratogenic in rats at doses that are maternally toxic. Under the conditions of this study, Carboxylic acid, C6-8 neo is not a selective developmental toxicant.</p>
Data Quality	<p>1 - Reliable without restrictions</p>
Reference	<p>Exxon Biomedical Sciences (1986) "Oral teratology study in rats," Unpublished study.</p>
Date last changed	<p>January, 2001</p>

Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>2,2-Dimethyloctanoic acid 26896-20-8</p> <p>Other Acute oral toxicity Pre-GLP 1964 Rats/Sprague-Dawley Males 5/dose Gastric Intubation None Single Dose 34.6, 120, 417, 1450, 5000, and 10000 mg/kg None</p> <p>The animals were fasted for a period of three to four hours prior to treatment. The animals were observed for toxic effects and mortality at one, four and 24 hours; and once daily thereafter for 14 days. Necropsy was performed on any animal that died. All surviving animals were weighed, sacrificed and necropsied.</p> <p>LD50= 2000 mg/kg</p> <p>There were no principal toxic effects or necropsy findings for animals in the 34.6, 120 and 417 mg/kg treatment groups. At 1450 mg/kg, 1 animal died within 24 hours of exposure and one animal died each day thereafter until all 5 animals were dead by day 5 of the study. Prior to death, slight to marked CNS depression, dyspnea, and ataxia was observed. In addition, congestion of the lungs, kidneys and adrenals were observed at necropsy. In the 5,000 mg/kg dose group, 2/5 animals died by 4 hours and 5/5 animals were dead by 24 hours following exposure. In the highest dose group, 4/5 animals died by 4 hours and all animals were dead by 24 hours post-treatment. Animals in the 5,000 and 10,000 mg/kg groups appeared to have depression, dyspnea, ataxia and sprawling of the limbs. Also at these two dose levels, necropsy findings indicated congestion of the lungs, liver, spleen, kidneys and adrenals.</p> <p>2,2-Dimethyloctanoic acid has a low order of acute oral toxicity in rodents.</p> <p>2 - Valid with restrictions (Pre-GLP)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>October, 2000</p>
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Robust Summaries - Neoacids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p>	<p>2,2-Dimethyloctanoic acid 26896-20-8</p> <p>NA Acute dermal toxicity Pre-GLP 1964 Albino Rabbits Males and Females 4/dose Dermal None Single Dose 50, 200, 794, 3160 mg/kg None</p> <p>Undiluted test sample was applied to clipped, intact abdominal skin under a dental dam binder. The trunk was subsequently wrapped with gauze and adhesive tape. Following a 24-hour exposure period, binders were removed and the abdominal area was sponged with corn oil to remove sample residue. Following exposure, animals were observed for mortality or toxic effects at 1, 4, and 24 hours, and once daily thereafter for a total of 14 days. A necropsy was performed on any animal that died during the study. At the end of the 14-day observation period, all surviving animals were weighed, sacrificed, and necropsied.</p>
<p>Results</p>	<p>LD50 > 3160 mg/kg</p>
<p>Remarks</p>	<p>No deaths occurred with any of the doses tested. The animals appeared normal in appearance and behavior throughout the study. All of the animals exhibited a normal pattern of weight gain. No signs of gross pathology were observed at necropsy.</p> <p>No dermal irritation was observed at the 50 mg/kg dose level and minimal irritation characterized by slight erythema, atonia, and desquamation that subsided in 10 days was noted at the 200 mg/kg level. At the 794 and 3160 mg/kg levels, a dose-dependent increase in the degree of irritation was observed. This consisted of slight to moderate erythema, which subsided after the fourth and eighth days, and slight to moderate atonia and desquamation that diminished in severity through the 14-day period.</p>
<p>Conclusions</p>	<p>Under conditions of this study, 2,2-Dimethyloctanoic acid has a low order of acute dermal toxicity in rabbits.</p>
<p>Data Quality</p>	<p>2 - Valid with restrictions (Pre-GLP)</p>
<p>Reference</p>	<p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p>
<p>Date last changed</p>	<p>January, 2001</p>

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Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>2,2-Dimethyloctanoic acid 26896-20-8</p> <p>Other Acute inhalation toxicity Pre-GLP 1964 Rats/Wistar, Mice/Swiss albino Males 10/species Inhalation None Single 6-hour exposure Saturated vapors - the mean nominal concentration was 3.0 mg/L. A group of mice and rats that served as a common control for the substances tested in this study were sacrificed and examined grossly.</p> <p>An atmosphere of saturated vapors was produced by forcing air through a bubbler system that contained the test substance. 20 ml of liquid was vaporized at a flow rate of 21 L/min. Animals were caged in wire mesh compartments within the exposure chamber. Animals were observed for mortality and toxic effects at 30-minute intervals during exposure and daily thereafter. The animals were observed for two weeks following exposure, at which point animals were sacrificed and necropsied. Any animals that died during the exposure or observation periods were also necropsied.</p> <p>LD50 > 3.0 mg/L</p> <p>No mortality or significant signs of toxicity were observed during the 6-hour exposure period. No deaths occurred in mice or rats throughout the study and no significant observations were made at necropsy.</p> <p>Under conditions of this study, 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice and rats.</p> <p>2 - Valid with restrictions - No vapor concentration verification (analytical)</p> <p>Esso Research and Engineering Company (1964). Acute Oral, Dermal, Eye Irritation and Inhalation Toxicity. Unpublished report.</p> <p>January, 2001</p>
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Robust Summaries - Neocids C5-C28

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment</p> <p>Remarks on Test Conditions</p>	<p>2,2-Dimethyloctanoic acid 26896-20-8</p> <p>Other Acute inhalation toxicity No 1982 Rats/Wistar, Mice/Swiss albino, Guinea Pigs/Harley Males and Females 10/sex/species Inhalation None Single 6-hour exposure Liquid aerosol with a mean analytical concentration of 511 mg/m³ 10/sex/species</p> <p>Groups of animals (10/sex/species) were exposed to either air only or to aerosolized test material. Aerosol was generated by pumping the test material into an atomizer at 15.0 psi. The resulting aerosol was sprayed into a glass aerosol diffuser, where it was mixed with incoming room air before entering the chamber. Exposure concentrations were determined on both a nominal and actual (gravimetric) basis. Particle size determinations were conducted twice during exposure. During the exposure, control and treated animals were observed every 15 minutes for the first hour and hourly thereafter. On the first day post-exposure, one half of the animals from each group were randomly selected and sacrificed, and an interim necropsy was performed. The remaining animals were observed daily for signs of toxicity for 14 days post-exposure. Body weights were recorded at the beginning of the study, and at 1, 2, 3, 4, 7, and 14 days post-exposure. A necropsy was performed on all animals that died or were sacrificed during the study. Major organs were examined for macroscopic abnormalities and lungs plus trachea, liver, kidneys, whole head, and any abnormal tissues were preserved. Organ weights were recorded at necropsy for lungs plus trachea, liver, and kidneys.</p>
<p>Results</p>	<p>LD50 > 511 mg/m³</p>
<p>Remarks</p>	<p>No animals died during the study. The control animals appeared normal throughout the exposure. During the two-week post-exposure period, incidences of ungroomed appearance, soft stool, and anogenital staining were observed in some of the control animals. One female guinea pig in the control group died on the fifth day of the post-exposure observation period.</p> <p>Animals exposed to the test material exhibited some signs of labored breathing, salivation, and eye irritation during the exposure. Upon removal from the chamber, exposed mice and guinea pigs had material-covered fur and exposed rats had some red staining around the nasal area, anogenital staining, soft stool, salivation, and lacrimation. During the two-week post-exposure observation period, all guinea pigs appeared normal. However, some of the mice appeared ungroomed and some rats exhibited anogenital staining and soft stool. Throughout the study, body weights remained normal except for a slight weight loss on the first and second post-exposure days in both the control and treated groups (all species).</p>

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Results, continued	<p>At terminal sacrifice, male mice exposed to the aerosolized test substance exhibited a statistically significant decrease in the liver to body weight ratio versus control animals. No other statistically significant differences were observed for group mean organ weight to body weight ratios. Minor macroscopic abnormalities were observed in both control and treated groups at the interim and terminal necropsies, but were not considered to be related to exposure to the test substance.</p>
Conclusions	<p>Under conditions of this study, aerosolized 2,2-Dimethyloctanoic acid has a low order of acute inhalation toxicity in mice, rats, and guinea pigs.</p>
Data Quality	<p>1 - Valid without restrictions</p>
Reference	<p>Bio/dynamics, Inc. (1982) "Evaluation of the Acute inhalation Toxicity in Rats, Mice, and Guinea Pigs". Unpublished report.</p>
Date last changed	<p>January, 2001</p>

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Repeat Dose Toxicity

<p>Test Substance CAS No.</p> <p>Method Type of Study GLP Year Species/Strain</p> <p>Sex Number/sex/dose Route of administration Vehicle Exposure Period Concentrations Controls</p> <p>Statistical method</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks for Results</p>	<p>2,2-Dimethyloctanoic acid 26896-20-8</p> <p>Other Repeat dermal application Pre-GLP 1964 Albino Rabbits</p> <p>Male 4/dose Dermal None 10 applications with a two-day rest between the 5th and 6th applications. 0.4 g/kg and 2.28 g/kg Isopropyl Alcohol (IPA) was administered to 8 animals at a level of 2.5 ml/kg body weight per application. Not reported</p> <p>The test material was applied to clipped abdominal skin. A loose gauze binder or a collar was used to prevent ingestion of the test substance. Animals were housed individually and allowed free access to food and water. Each animal was weighed, sacrificed, and necropsied 24 hours after the final application of test material. At the beginning of the study and prior to the final application, the following clinical parameters were evaluated: total erythrocyte count, total and differential leukocyte count, hematocrit, and urinalysis. Histological analysis was performed on sections of liver and kidney. Sections of brain, thyroid, lungs, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved for possible future analysis.</p> <p>For systemic effects: NOAEL = 2.28 g/kg 2,2-Dimethyloctanoic acid produced moderate skin irritation.</p> <p>Wheezing was noted in one animal of the low dose group. However, the rest of the animals appeared normal in behavior and appearance throughout the study. Animals in the low dose group showed overall body weight gain while animals in the high dose group had a slight reduction in weight at the end of the study. Necropsy revealed parasitic areas on the liver and/or mesentery of three animals, emphysema in three animals, and fluid in the cranial cavity and sinuses of one animal. These findings, however, did not correlate with the dose of test material received and were not attributed to exposure to the test substance. Animals in both the low and high dose groups displayed a decrease in terminal total leukocyte count. However, these values were within the normal limit value for rabbits. Repeat applications did not cause any histopathological alterations to the liver or kidney of the rabbits.</p> <p>Animals in the low dose group displayed slight erythema and moderate atonia and desquamation starting on the first or fourth application and persisting through the remainder of the study. All animals in the high dose group had moderate erythema, moderate to marked atonia and desquamation, and slight edema after the fifth application. After seven applications, slight fissures were observed in some of the animals and the exposed skin became hypersensitive to touch.</p>
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Conclusions	Under the conditions of this study, 2,2-Dimethyloctanoic acid has a low order of systemic toxicity following subchronic dermal exposure.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Hazleton Laboratories, Inc. (1964) "Repeated Dermal Application - Rabbits," Unpublished report.
Date last changed	January 2001

Reproductive Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of Treatment Dose/Concentration Levels Control group and Treatment Duration of Test Pre-mating Exposure Period	2,2-Dimethyloctanoic acid 26896-20-8 Other Reproductive Toxicity Pre-GLP 1968 Rats/Sprague-Dawley Males and Females P ₁ : 80 females and 40 males Dietary Continuous 0, 100, 500, 1500 ppm in diet Purina Lab Chow, 0 ppm of test substance 3 generations P1: 9 weeks for both males and females
Remarks on Test Conditions	<p>Pre-mating Period: For each dose level, 10 males and 20 females comprised the P₁ generation. The parental generation animals were maintained in individual cages and fed the corresponding diet for 9 weeks prior to mating. Individual body weights, food consumption, and observations of the physical appearance and behavior of the animals were recorded initially, at 5 weeks, and 9 weeks (P₁), or at 8 weeks, and 12 weeks (P₂). The F2B weanlings (P₃) were fed the appropriate diets for 9 weeks and the same observations were recorded at 0, 8, and 9 weeks of exposure.</p> <p>Reproduction Period: Following 9 weeks of exposure, two females and 1 male from each group were housed together and allowed a 3-week mating period, during which time, males were rotated among the females on a weekly basis. 24 hours following birth of the F1A generation, litters were arbitrarily reduced to a maximum of 8 pups (4/sex) to be nursed. The number of conceptions, litters, live births, stillbirths, the size of natural and nursing litters, deaths during the period of lactation, and number of pups weaned were all recorded. The weights of the pups by sex were recorded at 24 hours and at weaning and all pups were observed for gross signs of abnormalities. Following the 21-day nursing period, representative pups from each litter were sacrificed and gross necropsies were performed. The remaining pups were discarded.</p> <p>One week following the weaning of the F1A litters, the P1 parents were re-mated in the same fashion to produce the F1B pups. Following the 21-day nursing period, 20 female and 10 male weanlings from each of the test groups were randomly designated as the P2 generation. The remaining F1B pups were sacrificed and necropsied. The P2 generation was fed the appropriate diet until 100 days of age and then mated in the same fashion to produce the F2A and F2B litters. The same procedures were followed as during the first reproductive phase. After the second litter, F2B, 20 females and 10 males were selected at random to be the P3 generation. Following 9 weeks of dietary administration to this generation, the study was terminated and gross necropsies were performed. The following tissues were preserved: brain, pituitary, eye, thyroid, lung, heart, liver, spleen, kidney, adrenal, stomach, pancreas, small and large intestine, urinary bladder, gonad, bone, bone marrow, and trachea. Tissues from 5 females and 5 males of the control and high dose groups underwent histological examination. In addition, sections of thyroid, lung, liver, kidney, adrenal and trachea from 5 females and 5 males of the low level and intermediate level groups were examined microscopically.</p>

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Results	NOAEL Parental: 1500 ppm NOAEL F1 Offspring: 1500 ppm NOAEL F2 Offspring: 1500 ppm
Remarks	<p>For all of the concentrations tested, no adverse effects were observed on survival, appearance, behavior, body weight gain, and food consumption in either the parental generation or either the F1 or F2 generations. In addition, the reproductive performance of the parents was not affected. No treatment-related gross or microscopic pathological findings were observed at any of the dietary levels.</p> <p>All of the P1 and P2 animals survived the pre-mating periods and all of the P3 animals survived the 9-week post-weaning period of exposure. The body weight gain, food consumption, appearance, and behavior of the rats in these test groups were comparable with that of the control rats. In the F1A and F1B litters, litter size, pup body weights, appearance, and behavior were comparable between the treated groups and the control group. There were a variety of incidental findings in pups of the F1A and F1B litters, however, pups of these litters did not display any signs of treatment-related toxicity. At necropsy, there were no gross alterations that could be attributed to exposure to the test substance. The F2A and F2B litters, similar to the F1 litters had incidental findings, but did not show any treatment-related signs of toxicity, or effects on litter size, pup body weights, appearance, or behavior. Examination of the F2B weanling pups also (P3) did not reveal any treatment-related abnormalities.</p>
Conclusions	Under the conditions of this study, dietary exposure to 2,2-Dimethyloctanoic acid has a low order of reproductive toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Hazleton Labs, Inc. (1968) "Modified Three-Generation Reproduction Study - Rats," Unpublished report.
Date last changed	January 2001

Robust Summaries - Neoacids C5-C28

Developmental Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle: Dose/Concentration Levels Control group and Treatment Statistical methods</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p>	<p>Isooctanoic Acid 25103-52-0</p> <p>Other Developmental Toxicity Yes 1995 Rat/Sprague-Dawley Female 25/dose Oral gavage Corn oil 0, 50, 200, 400, 800, and 1000 mg/kg/day Vehicle control: corn oil Statistical evaluation of equality of means was done by appropriate one way analysis of variance. Also, a standard regression analysis for linear response in the dose groups was performed.</p> <p>Males and females were housed together until confirmation of mating. The presence of a sperm plug was set as gestational day (GD) 0. Mated females were dosed once daily from GD 6-15. Dosing volumes were 5 ml/kg for all groups and were based on the most recent body weight. Clinical observations were made daily during gestation. Food consumption and body weight measurements were made on every three days through GD21. On GD21, animals were euthanized and cesarean sections were performed. Gross necropsies were performed, uterine weights with ovaries were measured, uterine contents were examined, and uterine implantation data were recorded. All live fetuses were weighed, examined externally to determine sex and for gross malformations.</p> <p>Maternal NOAEL = 400 mg/kg/day Fetal NOAEL = 800 mg/kg/day</p> <p>Maternal: There were no treatment-related deaths during the study. However, there were some deaths in the different dose groups that were attributed to intubation errors. Animals in the 800 and 1000 mg/kg/day groups displayed clinical signs that included rales, stool abnormalities, and anogenital/abdominal staining following dose initiation on GD6. Animals in the remaining dose groups were free of clinical signs for the entire gestation period. Overall, there were no statistically significant differences in mean body weight gain for the entire gestation interval or the entire gestation interval corrected for uterine weight between treated and control animals. However, in the 800 and 1000 mg/kg/day groups, there were statistically significant decreases in body weight gain early during gestation (GD 6-15). This correlated with decreased mean food consumption in these groups during this time frame. In the 400 mg/kg/day group, there was evidence of slight body weight gain suppression during the interval following dosing. However, these animals recovered quickly and in the absence of a consistent response, this finding was considered the result of slight dosing trauma. There were no significant findings at necropsy other than some trauma that was indicative of dosing errors.</p>
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<p>Results, continued</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Fetal: There were no statistically significant differences in reproductive parameters including: total live fetuses, sex ratio, mean number of resorptions, mean number of implantation sites, mean number of corpora lutea, mean fetuses per implantation site, mean resorptions per implantation site, % pre-implantation losses, % post-implantation loss, or mean total affected (resorptions + dead + malformed fetuses per litter) between treated and control animals. No external abnormalities were observed in any fetuses from the control or treated groups. In the highest dose group, a statistically significant decrease in mean male and female fetal body weights was observed compared with the controls.</p> <p>Under the conditions of this study, Isooctanoic acid is not a selective developmental toxicant.</p> <p>2- reliable with restrictions - range-finding study.</p> <p>Exxon Biomedical Sciences, Inc. (1995). "Developmental toxicity range-finding study in rats," Unpublished report.</p> <p>October 22, 2001</p>
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Reproductive Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Dose/Concentration Levels Control group and Treatment Statistics</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p>	<p>Isooctanoic Acid 25103-52-0</p> <p>Other One-Generation Reproductive Toxicity Yes 1999 Rat/Sprague-Dawley Males and Females 10/sex/dose Dietary 0, 1000, 5000, 7500, and 10,000 ppm in diet 10/sex</p> <p>For the statistical analysis the percent of normal sperm were transformed by Bloom's transformation. All variables were analyzed by standard one-way analysis of variance (ANOVA). Residuals from the model were tested for normality by the Shapiro-Wilk. When there were differences in-group means based on the ANOVA, differences in means were tested using Duncan's multiple range test.</p> <p>P1 males and females (10 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were paired for up to 2 weeks. Beginning on GD 21, mated females were examined at least twice daily for signs of parturition. On PND 0, 1, 4, 7, 14 and 21 the offspring were counted, sexed and each live pup was weighed. Pups were counted and examined externally on a daily basis during the postnatal period. All animals were weighed and examined on PND 28, 35, 42, and 49 (males only were weighed and examined on PND Day 49). On PND 4, after counting, weighing, and examining the pups, the size of each litter was adjusted by eliminating extra pups by random selection to yield as nearly as possible, 4 males and 4 females per liter. Pups from each litter were examined daily for developmental landmarks. Sperm analyses were conducted at necropsy.</p> <p>Surviving F1 females were sacrificed on PND 42 and surviving F1 males were sacrificed on PND 49 unless they had not met criteria for vaginal patency or preputial separation, respectively.</p> <p>Maternal and Offspring NOAEL = 7500 ppm</p> <p>There were signs of a slight palatability problem with the 7500 ppm and 10,000 ppm diets with the males and the 10,000 ppm diet with the females as indicated by decreases in mean food consumption during the early part of the first week of the study. This problem resolved itself by the second week of the study. However, during the first week of gestation and for the entire postpartum period, mean food consumption was significantly decreased in the 10,000 ppm group females. There were no treatment-related clinical in-life observations, gross postmortem observations, or organ weight effect in the parental animals during this study. In addition, there were no statistically significant effects on reproductive indices or sperm parameters. The offspring displayed no treatment-related effects on survival, clinical observations, time to developmental landmarks, or offspring postmortem observations.</p> <p>Statistically significant suppression of body weight gain was observed in the 10,000 ppm adult females on PPD 4 and 14 when compared with controls. There were statistically significant decreases in the 10,000 ppm group's male mean offspring body weights on PND 14, 21, and 28. There also was a statistically significant decrease in the 10,000 ppm females' mean offspring body weight on PND 14 and 28. These decreases in body weight in dams and offspring were transient and were thought to be related to decreased maternal food consumption.</p>
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Conclusions	Under the conditions of this study Isooctanoic acid did not adversely affect reproductive parameters at doses that were nontoxic to the dams or their offspring.
Data Quality	1 - Reliable without restrictions
Reference	Exxon Biomedical Sciences, Inc. (1999) "One generation reproduction toxicity range-finding study in rats," Unpublished report.
Date last changed	August, 2001

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Reproductive Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Dose/Concentration Levels Control group and Treatment</p>	<p>Isononanoic Acid 3302-10-1</p> <p>Other One-Generation Reproductive Toxicity Yes 1998 Rat/Sprague-Dawley Males and Females 10/sex/dose Dietary 0, 600, 1200, 2500, 5000 ppm in diet 10/sex</p>
<p>Statistics</p>	<p>For the statistical analysis the percent of normal sperm were transformed by Bloom's transformation. All variables were analyzed by standard one-way analysis of variance (ANOVA). Residuals from the model were tested for normality by the Shapiro-Wilk. When there were differences in-group means based on the ANOVA, differences in means were tested using Duncan's multiple range test.</p>
<p>Remarks on Test Conditions</p>	<p>P1 males and females (10 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were paired for up to 2 weeks. Beginning on GD 21, mated females were examined at least twice daily for signs of parturition. On PND 0, 1, 4, 7, 14, 21 and 28 the offspring were counted, sexed and each live pup was weighed. Pups were counted and examined externally on a daily basis during the postnatal period. On PND 4, after counting, weighing, and examining the pups, the size of each litter was adjusted by eliminating extra pups by random selection to yield as nearly as possible, 4 males and 4 females per litter. Pups from each litter were examined daily for developmental landmarks. Sperm analyses were conducted at necropsy. Surviving F1 females were sacrificed on PND 42 and surviving F1 males were sacrificed on PND 49 unless they had not met criteria for vaginal patency or preputial separation, respectively.</p>
<p>Results</p>	<p>Maternal and Offspring NOAEL = 1200 ppm</p>
<p>Remarks</p>	<p>There were no treatment-related deaths or clinical signs noted in the parental animals during this study. There also were no treatment-related clinical signs noted for the offspring. There were no treatment-related effects noted for the male reproductive parameters such as sperm motility, total cauda sperm count, homogenization resistant spermatid count, sperm morphology, or the reproduction indices of mean male fertility, male mating, female fertility, fecundity, or gestational indices. In addition, there were no treatment-related effects on absolute or relative reproductive organ weights.</p> <p>In the 5000 ppm dose group, statistically significant decreases in parental food consumption were attributed to reduced palatability of the diet. Decreases in body weights were noted in the 5000 ppm females at Gestation Days (GD) 7 and 21 and at Postpartum Days (PPD) 4, 7, and 14. Mean absolute and mean relative liver weights were increased in both sexes of the 5000 ppm group.</p> <p>The offspring of the 5000 ppm group had reduced Live Birth Index and reduced survival indices on Day 1 and Day 4. Also, offspring body weights of both sexes were reduced during the postnatal period. Offspring body weight was also reduced in males and female of the 2500 ppm group.</p>

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Conclusions	Under the conditions of this study the test substance did not adversely affect reproductive parameters at doses that were nontoxic to the dams or their offspring.
Data Quality	1 - Reliable without restrictions
Reference	Exxon Biomedical Sciences, Inc. (1998) "One generation reproduction toxicity range-finding study in rats," Unpublished report.
Date last changed	August, 2001