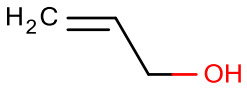
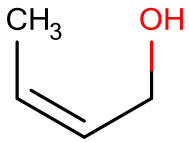
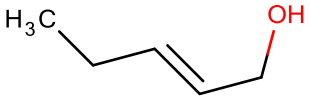
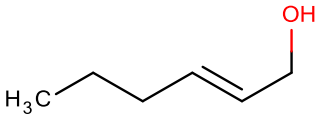
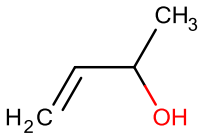
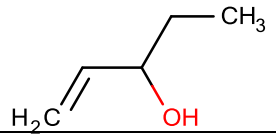
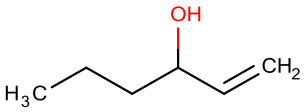
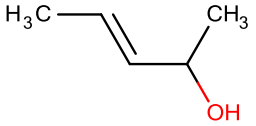
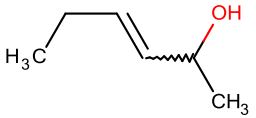
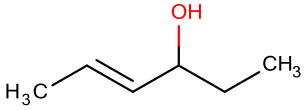
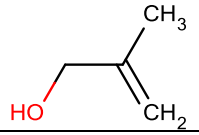
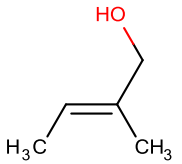
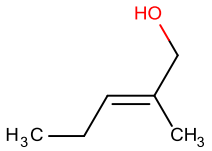
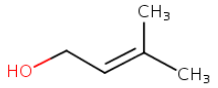
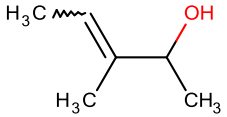
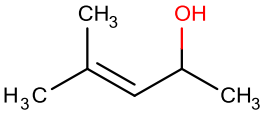
**Annex I Tables for Assessing Similarity of Analogues and Category Members for Read-Across[a]**

[a] Un-shaded analogues are considered part of the category. Data for shaded analogue reduce uncertainty and add weight-of-evidence.

**Table 1: Comparison of Substance Identification, Structure and Chemical Classifications**

| ID | Name | CAS No: | SMILES | 2D Structure | Molecular Formula: |
|---|---|---|---|---|---|
| 1 | 1-propen-3-ol | 107-18-6 | C(CO)=C |  | $C_3H_6O$ |
| 2 | 2-buten-1-ol | 6117-91-5 | OCC=CC |  | $C_4H_8O$ |
| 3 | 2-penten-1-ol | 20273-24-9 | CCC=CCO |  | $C_5H_{10}O$ |
| 4 | 2-hexen-1-ol | 2305-21-7 | CCCC=CCO |  | $C_6H_{12}O$ |
| 5 | 1-buten-3-ol | 598-32-3 | CC(C=C)O |  | $C_4H_8O$ |

| ID | Name | CAS No: | SMILES | 2D Structure | Molecular Formula: |
|---|---|---|---|---|---|
| 6 | 1-penten-3-ol | 616-25-1 | CCC(C=C)O |  | $C_5H_{10}O$ |
| 7 | 1-hexen-3-ol | 4798-44-1 | CCCC(C=C)O |  | $C_6H_{12}O$ |
| 8 | 3-penten-2-ol | 1569-50-2 | CC=CC(C)O |  | $C_5H_{10}O$ |
| 9 | 3-hexen-2-ol | 42185-97-7 | CC(O)C=CCC |  | $C_6H_{12}O$ |
| 10 | 4-hexen-3-ol | 4798-58-7 | CCC(C=CC)O |  | $C_6H_{12}O$ |
| 11 | 2-methyl-2-propen-1-ol | 513-42-8 | CC(=C)CO |  | $C_4H_8O$ |

| ID | Name | CAS No: | SMILES | 2D Structure | Molecular Formula: |
|---|---|---|---|---|---|
| 12 | 2-methyl-2-buten-1-ol | 4675-87-0 | CC=C(C)CO |  | $C_5H_{10}O$ |
| 13 | 2-methyl-2-penten-1-ol | 1610-29-3 | CCC=C(C)CO |  | $C_6H_{12}O$ |
| 14 | 3-methyl-2-buten-1-ol | 556-82-1 | CC(=CCO)C |  | $C_5H_{10}O$ |
| 15 | 3-methyl-3-penten-2-ol | 2747-53-7 | CC(O)C(C)=CC |  | $C_6H_{12}O$ |
| 16 | 4-methyl-3-penten-2-ol | 4325-82-0 | CC(O)C=C(C)C |  | $C_6H_{12}O$ |

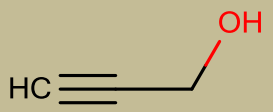
| ID | Name | CAS No: | SMILES | 2D Structure | Molecular Formula: |
|---|---|---|---|---|---|
| 17 | 2-propyn-1-ol<br>(1-propyn-3-ol ) | 107-19-7 | C#CCO |  | $C_3H_4O$ |

**Table 2: Comparison of Physico-Chemical and Molecular Properties[1]**

| ID | Name | **Molecular Weight** | **Log Kow**[a] | **Vapor Pressure**[b] [Pa at 25 deg C] | **Density**[d] [g/cm$^3$] | **Melting Point** [b] [deg C] | **Water Solubility**[c] | **Boiling Point**[b] [deg C] | **pKa**[e] |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1-propen-3-ol | 58.08 | 0.21<br>0.17 (M) | 3.12x10$^3$<br>3.48x10$^3$(M) | 0.8±0.1 | -76.37<br>-129 (M) | 3.177 x10$^5$<br>1 x10$^6$ (M) | 88.13<br>97 (M) | 14.43 |
| 2 | 2-buten-1-ol | 72.11 | 0.63 | 794 | 0.8±0.1 | -62.76<br><-30 (M) | 1.272 x10$^5$<br>1.66 x10$^5$ (M) | 121.10<br>123 (M) | 14.7 |
| 3 | 2-penten-1-ol | 86.13 | 1.12 | 351 | 0.8±0.1 | -50.48 | 4.572 x10$^4$ | 143.87<br>138 (M) | 14.7 |
| 4 | 2-hexen-1-ol | 100.16 | 1.61 | 121 | 0.8±0.1 | -38.47 | 1.6 x10$^4$ | 165.73<br>157 (M) | 14.45 |
| 5 | 1-buten-3-ol | 72.11 | 0.63 | 3.29x10$^3$ | 0.8±0.1 | -77.70 | 1.259 x10$^4$ | 89.94<br>96-97 (M) | 14.49 |
| 6 | 1-penten-3-ol | 86.13 | 1.12 | 1.22x10$^3$ | 0.8±0.1 | -65.08 | 4.526 x10$^4$<br>9.01 x10$^4$ (M) | 113.89<br>115 (M) | 14.49 |
| 7 | 1-hexen-3-ol | 100.16 | 1.61 | 437 | 0.8±0.1 | -52.76 | 1.58 x10$^4$<br>2.52 x10$^4$ (M) | 136.94<br>134 (M) | 14.49 |
| 8 | 3-penten-2-ol | 86.13 | 1.04 | 802 | 0.8±0.1 | -64.13 | 5.283 x10$^4$<br>8.92 x10$^4$ (M) | 122.82 | 14.77 |
| 9 | 3-hexen-2-ol | 100.16 | 1.53 | 231 | 0.8±0.1 | -51.87 | 1.849 x10$^4$ | 145.52 | 14.77 |
| 10 | 4-hexen-3-ol | 100.16 | 1.53 | 231 | 0.8±0.1 | -51.87 | 1.849 x10$^4$<br>3.81 x10$^4$ (M) | 145.52 | 14.77 |
| 11 | 2-methyl-2-propen-1-ol | 72.11 | 0.76 | 199 | 0.8±0.1 | -72.59 | 9.757 x10$^4$<br>1.94 x10$^5$ (M) | 105.69 | 14.49 |
| 12 | 2-methyl-2-buten-1-ol | 86.13 | 1.17 | 356 | 0.8±0.1 | -59.25 | 4.094 x10$^4$ | 137.75 | 14.87 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 13 | 2-methyl-2-penten-1-ol | 100.16 | 1.66 | 66.7 | 0.8±0.1 | -47.16 | 1.433 x$10^4$ | 159.86<br>167.5 (M) | 14.86 |
| 14 | 3-methyl-2-buten-1-ol | 98.1 | 1.17 | 314 | 0.8±0.1 | -59.25 | 4.094 x$10^4$ | 137.75<br>140 (M) | 14.83 |
| 15 | 3-methyl-3-penten-2-ol | 100.16 | 1.59 | 325 | 0.8±0.1 | -60.63 | 1.655 x$10^4$ | 139.41 | 14.94 |
| 16 | 4-methyl-3-penten-2-ol | 100.16 | 1.59 | 325 | 0.8±0.1 | -60.63 | 1.655 x$10^4$ | 139.41 | 14.9 |
| 17 | 2-propyn-1-ol (1-propyn-3-ol ) | 56.06 | -0.42<br>-0.38 (M) | 1.31x$10^3$<br>2.08x$10^3$(M) | 0.9±0.1 | -48.98<br>-51.8 (M) | 9.355 x$10^5$<br>1x$10^6$ (M) | 98.47<br>113.6 (M) | 13.21 |

[1]Values typically derived from EPISuite v4.1; [a] KOWWIN Program (v1.68); [b] MPBPWIN v1.43; [c] at 25 deg C (mg/L) Kow (WSKOW v1.42); [d] ACD/Lab Percepta Platform - PhysChem Module (from ChemSpider); [e] ACD (Advanced Chemistry Development Inc., Toronto, Canada)
(M): measured: Hansch, C et al. (1995); Yalkowsky, SH & Dannenfelser, RM (1992); Beilstein;

**Table 3: Comparison of Substituents, Functional Groups, and Extended Structural Fragments**

| ID | Name | Key Substituent(s) | Functional Group(s) | Extended Fragment(s) | Chemical Class: | Chemical Sub-Class: |
|---|---|---|---|---|---|---|
| 1 | 1-propen-3-ol | β-Olefin (C=C) | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 2 | 2-buten-1-ol | β-Olefin (C=C) | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 3 | 2-penten-1-ol | β-Olefin (C=C) | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 4 | 2-hexen-1-ol | β-Olefin (C=C) | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 5 | 1-buten-3-ol | β-Olefin (C=C) | Internal hydroxyl | | β-unsaturated alcohols | secondary allylic |
| 6 | 1-penten-3-ol | β-Olefin (C=C) | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 7 | 1-hexen-3-ol | β-Olefin (C=C) | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 8 | 3-penten-2-ol | β-Olefin (C=C) | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 9 | 3-hexen-2-ol | β-Olefin (C=C) | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 10 | 4-hexen-3-ol | β-Olefin (C=C) | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 11 | 2-methyl-2-propen-1-ol | β-Olefin (C=C) Methyl | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 12 | 2-methyl-2-buten-1-ol | β-Olefin (C=C) Methyl | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 13 | 2-methyl-2-penten-1-ol | β-Olefin (C=C) Methyl | External hydroxyl | | β-unsaturated alcohols | primary allylic |
| 14 | 3-methyl-2-buten-1-ol | β-Olefin (C=C) Methyl | External hydroxyl | | β-unsaturated alcohols | primary allylic |

| | | | | | | |
|---|---|---|---|---|---|---|
| 15 | 3-methyl-3-penten-2-ol | β-Olefin (C=C) Methyl | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 16 | 4-methyl-3-penten-2-ol | β-Olefin (C=C) Methyl | Internal hydroxy | | β-unsaturated alcohols | secondary allylic |
| 17 | 2-propyn-1-ol (1-propyn-3-ol ) | β-Acetylene (C≡C) | External hydroxyl | | β-unsaturated alcohols | primary propargylic |

**Table 4: Comparison of Abiotic Transformation and Toxicokinetics**

| ID | Name | Abiotic Transformation | Toxicokinetics |
|---|---|---|---|
| 1 | 1-propen-3-ol | Photodegradation: half-life = 4.32 hrs; rate constant = 2.59x10-11 cm3/molecule-sec[a] | Rapidly metabolised to acrolein by alcohol dehydrogenase; can be further oxidised to carboxylic acids and finaly to $CO_2$; Tmax = 30-60 min[a]<br>Km= 0.05 mM (binding affinities for human alcohol dehydrogenase), V= 10.3 (turnover no. X active site$^{-1}$ X min$^{-1}$)[b] |
| 2 | 2-buten-1-ol | | Km= 0.01 mM (binding affinities for human alcohol dehydrogenase), V= 13.0 (turnover no. X active site-1 X min-1)[b] |
| 3 | 2-penten-1-ol | | |
| 4 | 2-hexen-1-ol | | Km= 0.003 mM (binding affinities for human alcohol dehydrogenase), V= 15.5 (turnover no. X active site-1 X min-1)[b] |
| 5 | 1-buten-3-ol | | |
| 6 | 1-penten-3-ol | | |
| 7 | 1-hexen-3-ol | | |
| 8 | 3-penten-2-ol | | |
| 9 | 3-hexen-2-ol | | |
| 10 | 4-hexen-3-ol | | |
| 11 | 2-methyl-2-propen-1-ol | | |
| 12 | 2-methyl-2-buten-1-ol | | |
| 13 | 2-methyl-2-penten-1-ol | | |

| | | | |
|---|---|---|---|
| 14 | 3-methyl-2-buten-1-ol | | Km= 0.0045 mM (binding affinities for human alcohol dehydrogenase), V= 13.0 (turnover no. X active site-1 X min-1)[b] |
| 15 | 3-methyl-3-penten-2-ol | | |
| 16 | 4-methyl-3-penten-2-ol | | |
| 17 | 2-propyn-1-ol (1-propyn-3-ol ) | | Km= 6.7 (binding affinities for alcohol dehydrogenase) Vm= 0.050 $s^{-1}$ [c] |

[a] OECD SIDS Allyl Alcohol; [b] Pietruszko, R., Crawford, K. & Lester, D. 1973. Arch. Biochem. Biophys., 159, 50-60; [c] Moridani, M.Y., Khan, S., Chan, T., Teng, S., Beard, K. and Peter J. O'Brien, P.J. 2001. Chem.-Biol. Interact. 130-132: 931-942.

**Table 5: Comparison of Potential Metabolic Products**

| ID | Name | Liver metabolism simulator Toolbox v3.3.5 | | MetaPrint2D-React software | SMARTCyp version 2.4.2 | Meteor Nexus |
|---|---|---|---|---|---|---|
| | | Rat liver S9 | Skin metabolism | | | |
| 1 | 1-propen-3-ol | Oxidation (1) | Oxidation (1) | Epoxidation<br>Oxidation | Possible sites of metabolism | Epoxidation (1)<br>Oxidation (1) |
| 2 | 2-buten-1-ol | Hydroxylation (1)<br>Oxidation (1) | Oxidation (1) | Hydroxylation<br>Oxidation<br>Epoxidation<br>Acylation | Possible sites of metabolism | Hydroxylation (1)<br>Oxidation (1)<br>Epoxidation (1) |
| 3 | 2-penten-1-ol | Hydroxylation (1)<br>Oxidation (1) | Hydroxylation (1)<br>Oxidation (1) | Oxidation<br>Acylation | Possible sites of metabolism | Hydroxylation (2)<br>Oxidation (1)<br>Epoxidation (1) |
| 4 | 2-hexen-1-ol | Hydroxylation (2)<br>Oxidation (1) | Hydroxylation (2)<br>Oxidation (1) | Hydroxylation<br>Oxidation<br>Acylation | Possible sites of metabolism | Hydroxylation (3)<br>Oxidation (1)<br>Epoxidation (1) |
| 5 | 1-buten-3-ol | Oxidation (1) | Hydroxylation (1) | Epoxidation<br>Epoxidation/Hydrolysis | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (1)<br>Epoxidation (1) |
| 6 | 1-penten-3-ol | Hydroxylation (1)<br>Oxidation (1) | Hydroxylation (2) | Hydroxylation | Possible sites of metabolism | Hydroxylation (2)<br>Oxidation (1)<br>Epoxidation (1) |
| 7 | 1-hexen-3-ol | Hydroxylation (2)<br>Oxidation (1) | Hydroxylation (2) | Hydroxylation<br>Oxidation<br>Acetylation | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (3)<br>Epoxidation (1) |
| 8 | 3-penten-2-ol | Oxidation (1) | Hydroxylation (1) | Hydroxylation<br>Oxidation<br>Epoxidation | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (2)<br>Epoxidation (1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| 9 | 3-hexen-2-ol | Hydroxylation (1)<br>Oxidation (1) | Hydroxylation (2) | Hydroxylation<br>Oxidation<br>Alkylation | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (3)<br>Epoxidation (1) |
| 10 | 4-hexen-3-ol | Hydroxylation (2)<br>Oxidation (1) | Hydroxylation (2) | Hydroxylation<br>Oxidation<br>Acetylation | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (3)<br>Epoxidation (1) |
| 11 | 2-methyl-2-propen-1-ol | Oxidation (1) | No metabolism | No metabolism | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (1) |
| 12 | 2-methyl-2-buten-1-ol | Oxidation (1) | Hydroxylation (1) | Acetylation<br>Acylation | Possible sites of metabolism | Hydroxylation (2)<br>Oxidation (1)<br>Epoxidation (1) |
| 13 | 2-methyl-2-penten-1-ol | Hydroxylation (1)<br>Oxidation (1) | Hydroxylation (1) | Hydroxylation<br>Oxidation<br>Acetylation<br>Acylation<br>Dehydroxylation | Possible sites of metabolism | Hydroxylation (3)<br>Oxidation (1)<br>Epoxidation (1) |
| 14 | 3-methyl-2-buten-1-ol | Hydroxylation (1)<br>Oxidation (1) | No metabolism | Hydroxylation<br>Oxidation<br>Alkylation<br>Acylation | Possible sites of metabolism | Hydroxylation (2)<br>Oxidation (1)<br>Epoxidation (1) |
| 15 | 3-methyl-3-penten-2-ol | Oxidation (1) | Hydroxylation (2) | Hydroxylation<br>Oxidation<br>Acetylation | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (3)<br>Epoxidation (1) |
| 16 | 4-methyl-3-penten-2-ol | Oxidation (1) | Hydroxylation (1) | Hydroxylation<br>Oxidation<br>Alkylation | Possible sites of metabolism | Oxidation (1)<br>Hydroxylation (3)<br>Epoxidation (1) |
| 17 | 2-Propyn-1-ol<br>(1-Propyn-3-ol ) | Oxidation (1) | No metabolism | Oxidation | Possible sites of metabolism | Oxidation (1) |

() - The number of metabolites for specific transformation.

**Table 6A: Comparison of Toxicophores for β-unsaturated alcohols**

| ID | Name | Toxicophores[1] | Structural alerts[1,2] | | | | |
|---|---|---|---|---|---|---|---|
| | | | DNA binding by OECD[1] | Protein binding by OECD[1] | Protein binding potency (GSH)[1] | In vivo mutagenicity (Micronucleus) alerts by ISS[1] | Mitochondria toxicity[2] |
| 1 | 1-propen-3-ol | Cramer Class III | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 2 | 2-buten-1-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 3 | 2-penten-1-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 4 | 2-hexen-1-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 5 | 1-buten-3-ol | Cramer Class III | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 6 | 1-penten-3-ol | Cramer Class III | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 7 | 1-hexen-3-ol | Cramer Class III | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 8 | 3-penten-2-ol | Cramer Class II | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 9 | 3-hexen-2-ol | Cramer Class II | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 10 | 4-hexen-3-ol | Cramer Class II | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 11 | 2-methyl-2-propen-1-ol | Cramer Class III | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 12 | 2-methyl-2-buten-1-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |

| ID | Name | Toxicophores[1] | Structural alerts[1,2] | | | | |
|---|---|---|---|---|---|---|---|
| | | | DNA binding by OECD[1] | Protein binding by OECD[1] | Protein binding potency (GSH)[1] | In vivo mutagenicity (Micronucleus) alerts by ISS[1] | Mitochondria toxicity[2] |
| 13 | 2-methyl-2-penten-1-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 14 | 3-methyl-2-buten-1-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 15 | 3-methyl-3-penten-2-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 16 | 4-methyl-3-penten-2-ol | Cramer Class I | No alert | No alert | Not classified | No alert | Alert C=CCO |
| 17 | 2-propyn-1-ol | Cramer Class III | No alert | No alert | Not classified | No alert | No alert |

[1] OECD QSAR Toolbox 3.3.5; [2] COSMOS profiler available at: http://knimewebportal.cosmostox.eu/webportal

**Table 6B: Comparison of Toxicophores for metabolites**

| ID | Name | Toxicophores[1] | Structural alerts[1] | | | | |
|---|---|---|---|---|---|---|---|
| | | | DNA binding by OECD | Protein binding by OECD | Protein binding potency (GSH) | Carcinogenicity (genotox and nongenotox) alerts by ISS | *In vivo* mutagenicity (Micronucleus) alerts by ISS |
| 1 | 2-propenal (acrolein) | Cramer Class II | Michael addition | Michael addition, Schiff Base Formers | Extremely reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 2 | 2-butenal (crotonal dehyde) | Cramer Class I | Michael addition | Michael addition, Schiff Base Formers | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 3 | trans-2-pentenal | Cramer Class I | Michael addition | Michael addition, Schiff Base Formers | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 4 | trans-2-hexenal | Cramer Class I | Michael addition | Michael addition, Schiff Base Formers | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 5 | methyl vinyl ketone | Cramer Class II | Michael addition | Michael addition | Extremely reactive | Genotoxic carcinogenicity, α,β-unsaturated | α,β-unsaturated carbonyls |

| ID | Name | Toxicophores[1] | Structural alerts[1] | | | | |
|---|---|---|---|---|---|---|---|
| | | | DNA binding by OECD | Protein binding by OECD | Protein binding potency (GSH) | Carcinogenicity (genotox and nongenotox) alerts by ISS | *In vivo* mutagenicity (Micronucleus) alerts by ISS |
| | | | | | | carbonyls | |
| 6 | ethyl vinyl ketone | Cramer Class II | Michael addition | Michael addition | Extremely reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 7 | propyl vinyl ketone | Cramer Class II | Michael addition | Michael addition | Extremely reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 8 | 3-penten-2-one | Cramer Class I | Michael addition | Michael addition | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 9 | 3-hexen-2-one | Cramer Class I | Michael addition | Michael addition | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 10 | 4-hexen-4-one | Cramer Class I | Michael addition | Michael addition | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |

| ID | Name | Toxicophores[1] | Structural alerts[1] | | | | |
|---|---|---|---|---|---|---|---|
| | | | DNA binding by OECD | Protein binding by OECD | Protein binding potency (GSH) | Carcinogenicity (genotox and nongenotox) alerts by ISS | *In vivo* mutagenicity (Micronucleus) alerts by ISS |
| 11 | 2-methyl acrolein | Cramer Class II | Michael addition | Michael addition, Schiff Base Formers | Moderately reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 12 | 2-methyl-2-butenal | Cramer Class I | Michael addition | Michael addition, Schiff Base Formers | Moderately reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 13 | 2-methyl-2-pentenal | Cramer Class I | Michael addition | Michael addition, Schiff Base Formers | Moderately reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 14 | 3-methyl-2-butenal | Cramer Class I | No alert | Schiff Base Formers | Moderately reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 15 | 3-methyl-3-penten-2-one | Cramer Class I | Michael addition | Michael addition | Highly reactive | Genotoxic carcinogenicity, α,β-unsaturated carbonyls | α,β-unsaturated carbonyls |
| 16 | 4-methyl-3- | Cramer Class I | No alert | No alert | Highly reactive | Genotoxic | α,β-unsaturated |

| ID | Name | Toxicophores[1] | Structural alerts[1] | | | | |
|---|---|---|---|---|---|---|---|
| | | | DNA binding by OECD | Protein binding by OECD | Protein binding potency (GSH) | Carcinogenicity (genotox and nongenotox) alerts by ISS | *In vivo* mutagenicity (Micronucleus) alerts by ISS |
| | penten-2-one | | | | | carcinogenicity, α,β-unsaturated carbonyls | carbonyls |
| 17 | acetylenic aldehyde | Cramer Class III | No alert | Michael addition, Schiff Base Formers | Extremely reactive | Genotoxic carcinogenicity, simple aldehyde | Simple aldehyde |

[1] OECD QSAR Toolbox 3.3.5

**Table 7: Comparison of Mechanistic Plausibility and AOP-Related Event Data**

| ID | Name | Mechanistic Plausibility | Adverse Outcome Pathway or Mode of Toxic Action: | Molecular Initiating Event: | Key Event 1 etc.: | Key Event Relationship 1 etc.: | Other Mechanistically-Relevant Events |
|---|---|---|---|---|---|---|---|
| 1 | 1-propen-3-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 2 | 2-buten-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 3 | 2-penten-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 4 | 2-hexen-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 5 | 1-buten-3-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 6 | 1-penten-3-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 7 | 1-hexen-3-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 8 | 3-penten-2-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 9 | 3-hexen-2-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 10 | 4-hexen-3-ol | | Apoptosis or | Covalent binding of | | | Hepatotoxicity |

| ID | Name | Mechanistic Plausibility | Adverse Outcome Pathway or Mode of Toxic Action: | Molecular Initiating Event: | Key Event 1 etc.: | Key Event Relationship 1 etc.: | Other Mechanistically-Relevant Events |
|---|---|---|---|---|---|---|---|
| | | | necrosis | reactive metabolite with thiols | | | |
| 11 | 2-methyl-2-propen-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 12 | 2-methyl-2-buten-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 13 | 2-methyl-2-penten-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 14 | 3-methyl-2-buten-1-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 15 | 3-methyl-3-penten-2-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 16 | 4-methyl-3-penten-2-ol | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |
| 17 | 2-propyn-1-ol (1-propyn-3-ol ) | | Apoptosis or necrosis | Covalent binding of reactive metabolite with thiols | | | Hepatotoxicity |

**Table 8: Comparison of Toxicologically Relevant *In Vivo*, *In Vitro* and *Ex Vivo* Data**

| Name | 1-propen-3-ol | 2-buten-1-ol | 2-penten-1-ol | 2-hexen-1-ol | 1-buten-3-ol | 1-penten-3-ol | 1-hexen-3-ol | 3-penten-2-ol | 3-hexen-2-ol | 4-hexen-3-ol | 2-methyl-2-propen-1-ol | 2-methyl-2-buten-1-ol | 2-methyl-2-penten-1-ol | 3-methyl-2-buten-1-ol | 3-methyl-3-penten-2-ol | 4-methyl-3-penten-2-ol | 2-propyn-1-ol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Endpoint: NOAEL (Repeat dose toxicity)** | 3-11.6 (mg/kg bw/day)<br><br>20-400 (ppm)<br>12 ($mg/m^3$)<br>[1-5] | | | | | | | | | | | | | 65.4 -82.1 (mg/ kg bw/d ay)<br>[53] | | | 5-20 (mg/kg bw/day)<br><br>23 ($mg/m^3$)<br><br>[9] |
| **Endpoint: NOEL (Repeat dose toxicity)** | 1.37 (mg/kg/ day)<br><br>[6] | | | | | | | | | | | | | 14.4 -21 (mg/ kg bw/d ay)<br>[53] | | | 5 (mg/kg/da y)<br><br>[9] |
| **Endpoint: LOAEL (Repeat dose toxicity)** | 47 ($mg/m^3$) | | | | | | | | | | | | | 243. 8- 307.2 | | | |

| Name | 1-propen-3-ol | 2-buten-1-ol | 2-penten-1-ol | 2-hexen-1-ol | 1-buten-3-ol | 1-penten-3-ol | 1-hexen-3-ol | 3-penten-2-ol | 3-hexen-2-ol | 4-hexen-3-ol | 2-methyl-2-propen-1-ol | 2-methyl-2-buten-1-ol | 2-methyl-2-penten-1-ol | 3-methyl-2-buten-1-ol | 3-methyl-3-penten-2-ol | 4-methyl-3-penten-2-ol | 2-propyn-1-ol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 6-34 (mg/kg/day) [1, 4, 7] | | | | | | | | | | | | | (mg/kg bw/day) [53] | | | |
| **Endpoint: LOEL (Repeat dose toxicity)** | 4.8-87.1 (mg/kg/day) [2, 6, 8] | | | | | | | | | | | | | | | | 15 (mg/kg/day) [9] |
| **Endpoint: NOAEC (Repeat dose toxicity)** | | | | | | | | | | | | | | | | | 4- 25.3 (mg/L) [9, 10] |
| **Endpoint: NOEC (Repeat dose toxicity)** | | | | | | | | | | | | | | | | | 11 (mg/L) [9] |
| **Endpoint: NOAEL (** | 8 (mg/kg/day) | | | | | | | | | | | | | | | | 5-15 |

| Name | 1-propen-3-ol | 2-buten-1-ol | 2-penten-1-ol | 2-hexen-1-ol | 1-buten-3-ol | 1-penten-3-ol | 1-hexen-3-ol | 3-penten-2-ol | 3-hexen-2-ol | 4-hexen-3-ol | 2-methyl-2-propen-1-ol | 2-methyl-2-buten-1-ol | 2-methyl-2-penten-1-ol | 3-methyl-2-buten-1-ol | 3-methyl-3-penten-2-ol | 4-methyl-3-penten-2-ol | 2-propyn-1-ol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Reproductive toxicity)** | 48.2-58.4 ($mg/m^3$) [2, 3] | | | | | | | | | | | | | | | | (mg/kg/ day) [9] |
| **Endpoint: NOAEL ( Teratogenicity)** | 10 (mg/kg/ day) [11] | | | | | | | | | | | | | | | | |
| **Endpoint: LOAEL (Maternal toxicity)** | 10 (mg/kg/ day) [7] | | | | | | | | | | | | | | | | |
| **Endpoint: NOEL ( Reproductive toxicity)** | 40 (mg/kg/ day) [3] | | | | | | | | | | | | | | | | |
| **Endpoint: Carcinogenic/ Genotoxicity** | 5 x Negative [12-15] | | | | | | | | | | | | | | | | |

| Name | 1-propen-3-ol | 2-buten-1-ol | 2-penten-1-ol | 2-hexen-1-ol | 1-buten-3-ol | 1-penten-3-ol | 1-hexen-3-ol | 3-penten-2-ol | 3-hexen-2-ol | 4-hexen-3-ol | 2-methyl-2-propen-1-ol | 2-methyl-2-buten-1-ol | 2-methyl-2-penten-1-ol | 3-methyl-2-buten-1-ol | 3-methyl-3-penten-2-ol | 4-methyl-3-penten-2-ol | 2-propyn-1-ol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Endpoint:LC50 (Acute toxicity)** | 140-2130 ($mg/m^3$)<br>500 ($mg/m^3$/ 2H<br>75 (ppm/8 H)<br>50->400 (ppm)<br>[1, 5, 16-18] | | | | | | | | | | | | | | | | 2000-3000<br>(mg/kg)<br>873-1200<br>(ppm)<br>[16, 33, 39, 42] |
| **Endpoint:LD50 (Acute toxicity)** | 37 -105 (mg/kg)<br>[1,16, | 1084-793 (mg/kg) | | 3500 (mg/kg) | 50 (ppm) | 70 (mg/kg) | 450 (mg/kg) | | | | 2924 (ppm)<br>2-500 (mg/kg) | | 3 (mL/kg)<br>4920 (mg/kg) | 810-3900<br>(mg/kg) | | | 2.83-2000<br>(mg/kg)<br>[9, 16, 20, 33-41] |

| Name | | 1-propen-3-ol | 2-buten-1-ol | 2-penten-1-ol | 2-hexen-1-ol | 1-buten-3-ol | 1-penten-3-ol | 1-hexen-3-ol | 3-penten-2-ol | 3-hexen-2-ol | 4-hexen-3-ol | 2-methyl-2-propen-1-ol | 2-methyl-2-buten-1-ol | 2-methyl-2-penten-1-ol | 3-methyl-2-buten-1-ol | 3-methyl-3-penten-2-ol | 4-methyl-3-penten-2-ol | 2-propyn-1-ol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 18-22] | [23, 54] | | [24] | [19] | [25] | [26] | | | | [27] | | [28] | [29-32] | | | |
| **Endpoint: hepatic fibrosis** | | 64-76 (U/L) [44] | | | | | | | | | | | | | | | | |
| **Endpoint: Genotoxicity (AMES, Chromosomal abrration, gene mutation)** | | 6x Negative 5 x Positive [15, 45-50] | | | | | | | | | | | | | Negative [32] | | | 17x Negative 3 x Positive [9, 51] |
| **Toxcast [52]** | ATG_RARb_TRANS | 18 | | | | | | | | | | | | | | | | |
| | ATG_RARb_TRANS_perc | 18 | | | | | | | | | | | | | | | | |

| Name | | 1-propen-3-ol | 2-buten-1-ol | 2-penten-1-ol | 2-hexen-1-ol | 1-buten-3-ol | 1-penten-3-ol | 1-hexen-3-ol | 3-penten-2-ol | 3-hexen-2-ol | 4-hexen-3-ol | 2-methyl-2-propen-1-ol | 2-methyl-2-buten-1-ol | 2-methyl-2-penten-1-ol | 3-methyl-2-buten-1-ol | 3-methyl-3-penten-2-ol | 4-methyl-3-penten-2-ol | 2-propyn-1-ol |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | OT_SRC1_SRC1FXR_1440 | 26 | | | | | | | | | | | | | | | | |
| | Tox21_AhR_viability | 0.8 | | | | | | | | | | | | | | | | |
| | Tox21_AR_BLA_Agonist_ch1 | 0.6 | | | | | | | | | | | | | | | | |
| | Tox21_AR_LUC_MDAKB2_Antagonist_viability | 0.00122 | | | | | | | | | | | | | | | | |
| | Tox21_ELG1_LUC_Agonist_viability | 25 | | | | | | | | | | | | | | | | |
| | Tox21_TR_LUC_GH3_Antagonist_viability | 0.00122 | | | | | | | | | | | | | | | | |

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