Electronic Supplementary Information

# Environmental risk – based ranking of solvents by the combination of multimedia model and multi-criteria decision analysis.

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*Statement*: For the same data point different literature values can be found.* We tried to find the data originating from reliable sources, collecting preferably experimental data not modelled or estimated. Because of the literature data variability, it is possible to find (sometimes significantly) another values in various sources.

ESI Table 1. Parameters used for the assessment procedure.

| Chemical group | No. | Compound | molar weight [g/mole] | CAS number | Inhalation $LC_{50}$ [ppm] | POCP | fish $LC_{50}$ [mg $L^{-1}$] | log BCF | Biodegradability half-life [day] | Oral $LD_{50}$ [mg $kg^{-1}$] | EPA/IACR cancer class |
|---|---|---|---|---|---|---|---|---|---|---|---|
| hydrocarbons | 1 | pentane | 72 | 109-66-0 | 123000 | 39.5 | 10 | 0 | 3 | 5000 | 0 |
| | 2 | hexane | 86 | 110-54-3 | 48000 | 48.2 | 2.5 | 0.35 | 1 | 25000 | 0 |
| | 3 | cyclohexane | 84 | 110-82-7 | 34000 | 23 | 4.3 | 2.38 | 28 | 12700 | 0 |
| | 4 | heptane | 100 | 142-82-5 | 103000 | 49.4 | 375 | 2.53 | 7 | 5000 | 0 |
| | 5 | octane | 114 | 111-65-9 | 25260 | 46.1 | 100 | 3.289 | 7 | 5000 | 0 |
| | 6 | isooctane | 114 | 540-84-1 | 3100 | 45 | 0.1 | 2.36 | 1 | 5000 | 0 |
| | 7 | nonane | 128 | 111-84-2 | 3200 | 41.4 | 300 | 2.651 | 7 | 4000 | 0 |
| | 8 | decane | 142 | 124-18-5 | 2738 | 38.4 | 500 | 2.158 | 7 | 5000 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | 9 | undecane | 156 | 1120-21-4 | 844 | 38.4 | 1000 | 2.722 | 28 | 5000 | 0 |
| | 10 | dodecane | 170 | 112-40-3 | 284 | 31.1 | 1000 | 2.497 | 7 | 5000 | 0 |
| | 11 | benzene | 78 | 71-43-2 | 13000 | 21.8 | 5.9 | 1.5 | 6 | 930 | 10 |
| | 12 | toluene | 92 | 108-88-3 | 26000 | 63.7 | 7.63 | 1.954 | 3 | 5500 | 0 |
| | 13 | o-xylene | 106 | 95-47-6 | 6125 | 105.3 | 17 | 1.702 | 4 | 4300 | 0 |
| | 14 | m-xylene | 106 | 108-38-3 | 6700 | 47.4 | 11 | 1.764 | 24 | 5000 | 0 |
| | 15 | p-xylene | 106 | 106-42-3 | 5000 | 47.2 | 16 | 1.3 | 7 | 2100 | 0 |
| | 16 | styrene | 104 | 100-42-5 | 9500 | 14.2 | 10 | 1.13 | 28 | 5000 | 8 |
| alcohols | 17 | methanol | 32 | 67-56-1 | 64000 | 14 | 15400 | 0.65 | 1 | 1200 | 0 |
| | 18 | ethanol | 46 | 64-17-5 | 20000 | 39.9 | 14500 | -1.63 | 2 | 3450 | 0 |
| | 19 | 1-propanol | 60 | 71-23-8 | 68000 | 56.1 | 4480 | -1.07 | 3 | 1870 | 0 |
| | 20 | isopropanol | 60 | 67-63-0 | 16000 | 18.8 | 5000 | 0.5 | 1 | 3600 | 0 |
| | 21 | 1-butanol | 74 | 71-36-3 | 8000 | 62 | 1200 | -0.439 | 7 | 790 | 0 |
| | 22 | isobutanol | 74 | 67-63-0 | 8000 | 44.7 | 1220 | 0.5 | 7 | 2460 | 0 |
| | 23 | sec-butyl alcohol | 74 | 78-92-2 | 16500 | 44.7 | 3670 | 0.5 | 7 | 2193 | 0 |
| | 24 | tert-butyl alcohol | 74 | 76-65-0 | 3300 | 10.6 | 1940 | -1.45 | 7 | 2743 | 0 |
| | 25 | 1-pentanol | 88 | 71-41-0 | 6000 | 59.5 | 370 | 0.463 | 4 | 2200 | 0 |
| | 26 | 1-hexanol | 102 | 111-27-3 | 5000 | 45 | 98 | 0.711 | 5 | 720 | 0 |
| | 27 | 1-heptanol | 116 | 111-70-6 | 9333 | 45 | 38 | 1.09 | 20 | 5500 | 0 |
| | 28 | 1-octanol | 130 | 111-87-5 | 6500 | 45 | 13.3 | 1.6 | 30 | 3200 | 0 |
| | 29 | 1-nonanol | 144 | 143-08-8 | 6500 | 45 | 18 | 2.2 | 40 | 3560 | 0 |
| | 30 | allyl alcohol | 58 | 107-18-6 | 76 | 45 | 0.32 | 0.5 | 3 | 64 | 0 |
| | 31 | benzyl alcohol | 108 | 100-51-6 | 1000 | 45 | 10 | 0.602 | 5 | 1230 | 0 |
| | 32 | glycerol | 92 | 56-81-5 | n.a.[†] | 22 | 5800 | 0.5 | 4 | 25000 | 0 |
| | 33 | phenol | 94 | 108-95-2 | 82 | -119 | 12 | 2.2 | 2 | 270 | 0 |
| | 34 | o-cresol | 108 | 95-45-7 | 40 | 19 | 6.2 | 1.1 | 2 | 121 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | 35 | m-cresol | 108 | 108-39-4 | 160 | 19 | 8.9 | 3 | 2 | 242 | 0 |
| | 36 | p-cresol | 108 | 106-44-5 | 160 | 19 | 7.9 | 1.26 | 2 | 207 | 0 |
| ethers | 37 | diethyl ether | 74 | 60-29-7 | 32000 | 44.5 | 2560 | 0.73 | 1 | 1215 | 0 |
| | 38 | methyl – tert butyl ether | 88 | 1634-04-4 | 23500 | 15.2 | 672 | 1.5 | 500 | 4000 | 0 |
| | 39 | furan | 68 | 110-00-9 | 60 | 20 | 61 | 0.332 | 300 | 5 | 8 |
| | 40 | tetrahydrofuran | 72 | 109-99-9 | 18000 | 20 | 2160 | 0 | 40 | 1650 | 0 |
| aldehydes | 41 | ethanal | 44 | 75-07-0 | 13300 | 64.1 | 31 | 0.5 | 15 | 661 | 8 |
| | 42 | 1-propanal | 58 | 123-38-6 | 1110 | 17 | 14 | 0.5 | 11 | 1410 | 0 |
| | 43 | 1-butanal | 72 | 123-72-8 | 6400 | 17.1 | 16 | 0.5 | 5 | 5900 | 0 |
| | 44 | furfural | 96 | 98-08-1 | 100 | 17 | 32 | 0.5 | 5 | 65 | 0 |
| ketones | 45 | acetone | 58 | 67-64-1 | 21000 | -4 | 5540 | -0.187 | 3 | 3200 | 0 |
| | 46 | 2-butanone | 72 | 78-93-3 | 10900 | 37.3 | 3220 | 0 | 11 | 2737 | 0 |
| | 47 | 2-pentanone | 86 | 107-87-9 | 2000 | 17.8 | 1240 | 0.477 | 7 | 1600 | 7 |
| | 48 | 3-pentanone | 86 | 96-22-0 | 5000 | 16 | 1530 | 0.3 | 7.5 | 2140 | 0 |
| | 49 | methyl isobutyl ketone | 100 | 108-10-1 | 3000 | 49 | 720 | 0.5 | 11 | 2080 | 7 |
| | 50 | 2-hexanone | 100 | 591-78-6 | 8000 | 57.2 | 428 | 0.778 | 5 | 2590 | 0 |
| | 51 | 2-heptanone | 114 | 110-43-0 | 8000 | 59.9 | 130 | 0.39 | 21 | 1760 | 0 |
| | 52 | cyclohexanone | 98 | 108-94-1 | 8000 | 12 | 527 | 0.5 | 7 | 1620 | 0 |
| terpenes | 53 | d-limonene | 136 | 5989-27-5 | 5000 | 134 | 0.72 | 2.673 | 7 | 4400 | 0 |
| | 54 | p-cymene | 134 | 99-87-6 | 1750 | 100 | 48 | 2.457 | 14 | 4750 | 0 |
| | 55 | α-pinene | 136 | 80-56-8 | 1110 | 84 | 0.28 | 2.719 | 21 | 3700 | 0 |
| | 56 | β-pinene | 136 | 127-91-3 | 3500 | 70 | 1 | 2.503 | 21 | 4700 | 0 |
| organic acids | 57 | formic acid | 46 | 64-18-6 | 825 | 4 | 46 | 0 | 1 | 730 | 0 |
| | 58 | acetic acid | 60 | 64-19-7 | 16000 | 6 | 1000 | 0 | 2 | 3310 | 0 |
| | 59 | butyric acid | 88 | 107-92-6 | 2200 | 8 | 66.4 | 0.5 | 2 | 2940 | 0 |
| | 60 | isobutyric acid | 88 | 79-31-2 | 2800 | 8 | 228 | 0.5 | 3 | 226 | 0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| | 61 | valeric acid | 102 | 109-52-4 | 1000 | 8 | 39 | 0.5 | 4 | 600 | 0 |
| | 62 | hexanoic acid | 116 | 142-62-1 | 865 | 8 | 88 | 0.5 | 5 | 1900 | 0 |
| esters | 63 | ethyl acetate | 88 | 141-78-6 | 8000 | 10 | 350 | 1.48 | 5 | 5620 | 0 |
| | 64 | ethyl acrylate | 100 | 140-88-5 | 1414 | 18 | 4.6 | 0.316 | 18 | 800 | 8 |
| | 65 | butyl lactate | 146 | 138-22-7 | 840 | 18 | 75 | 0.5 | 10 | 5000 | 0 |
| | 66 | ethyl lactate | 188 | 97-64-3 | 1120 | 0 | 320 | 0.5 | 14 | 2500 | 0 |
| | 67 | methyl formate | 60 | 107-31-3 | 2120 | 0 | 120 | 0.5 | 2 | 1622 | 0 |
| | 68 | methyl acetate | 74 | 79-20-9 | 16200 | 5.9 | 300 | 0.5 | 21 | 5000 | 0 |
| | 69 | methyl laurate | 214 | 111-82-0 | 571 | 0 | 0.52 | 2.466 | 5 | 2000 | 0 |
| chlorinated | 70 | dichloromethane | 85 | 75-09-2 | 16000 | 2.3 | 193 | 0.7 | 10 | 1600 | 8 |
| | 71 | chloroform | 119 | 67-66-3 | 15000 | 0.4 | 14 | 0.8 | 28 | 908 | 8 |
| | 72 | carbon tetrachloride | 154 | 56-23-5 | 8000 | 15 | 24.3 | 1.47 | 250 | 2350 | 8 |
| | 73 | trichloroethene | 131 | 79-01-6 | 8450 | 32.5 | 3.1 | 1.23 | 180 | 2400 | 10 |
| | 74 | tetrachloro-ethene | 166 | 127-18-4 | 4100 | 1.4 | 9.8 | 1.69 | 230 | 2629 | 8 |
| | 75 | 1,2-dichloro-ethane | 111 | 542-75-6 | 950 | 15 | 2.94 | 0.863 | 28 | 250 | 7 |
| | 76 | 1,3-dichloro-propene | 261 | 87-68-3 | 34 | 15 | 0.14 | 4.7 | 205 | 82 | 7 |
| | 77 | hexachlorobutadiene | 99 | 107-06-2 | 1414 | 15 | 136 | 0.3 | 180 | 413 | 7 |
| others | 78 | acetonitrile | 41 | 75-05-8 | 3587 | 25 | 1640 | 0.3 | 28 | 1320 | 0 |

IARC cancer class was translated into the numerical values in the following way: Group 1 (human carcinogen) – 10; Group 2A (probable human carcinogen) – 8; Group 2B (possible human carcinogen) – 7; Groups 3 and 4 (not classifiable and probable human noncarcinogen, respectively) – 0.

Notes and references:

[*] C.M. Alder, J. D. Hayler, R.K. Henderson, A.M. Redman, L. Shukla, L.E. Shuster, H.F. Sneddon, Green Chem. 2016,18, 3879-3890.

[†] Not needed as glycerol does not partition to air