DATA ENTRY SHEET

SL-ADV
Version 3.1; 02/04

Reset to Defaults

CALCULATE RISK-BASED SOIL CONCENTRATION (enter "X" in "YES" box)

YES: X

**OR**

CALCULATE INCREMENTAL RISKS FROM ACTUAL SOIL CONCENTRATION (enter "X" in "YES" box and initial soil conc. below)

YES:

| ENTER Chemical CAS No. (numbers only, no dashes) | ENTER Initial soil conc., $C_R$ (µg/kg) | Chemical |
|---|---|---|
| 98066 | | tert-Butylbenzene |

MORE ↓

| ENTER Average soil temperature, $T_S$ (°C) | ENTER Depth below grade to bottom of enclosed space floor, $L_F$ (cm) | ENTER Depth below grade to top of contamination, $L_t$ (cm) | ENTER Depth below grade to bottom of contamination, (enter value of 0 if value is unknown) $L_b$ (cm) | ENTER Totals must add up to value of $L_t$ (cell G28) Thickness of soil stratum A, $h_A$ (cm) | ENTER Thickness of soil stratum B, (Enter value or 0) $h_B$ (cm) | ENTER Thickness of soil stratum C, (Enter value or 0) $h_C$ (cm) | ENTER Soil stratum A SCS soil type (used to estimate soil vapor permeability) | OR | ENTER User-defined stratum A soil vapor permeability, $k_v$ ($cm^2$) |
|---|---|---|---|---|---|---|---|---|---|
| 10 | 15 | 610 | 640 | 610 | 0 | 0 | | | 1.00E-08 |

MORE ↓

| ENTER Stratum A SCS soil type | ENTER Stratum A soil dry bulk density, $\rho_b^A$ ($g/cm^3$) | ENTER Stratum A soil total porosity, $n^A$ (unitless) | ENTER Stratum A soil water-filled porosity, $\theta_w^A$ ($cm^3/cm^3$) | ENTER Stratum A soil organic carbon fraction, $f_{oc}^A$ (unitless) | ENTER Stratum B SCS soil type | ENTER Stratum B soil dry bulk density, $\rho_b^B$ ($g/cm^3$) | ENTER Stratum B soil total porosity, $n^B$ (unitless) | ENTER Stratum B soil water-filled porosity, $\theta_w^B$ ($cm^3/cm^3$) | ENTER Stratum B soil organic carbon fraction, $f_{oc}^B$ (unitless) | ENTER Stratum C SCS soil type | ENTER Stratum C soil dry bulk density, $\rho_b^C$ ($g/cm^3$) | ENTER Stratum C soil total porosity, $n^C$ (unitless) | ENTER Stratum C soil water-filled porosity, $\theta_w^C$ ($cm^3/cm^3$) | ENTER Stratum C soil organic carbon fraction, $f_{oc}^C$ (unitless) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Lookup Soil Parameters | | | | | Lookup Soil Parameters | | | | | Lookup Soil Parameters | | | | |
| | 1.65 | 0.439 | 0.045 | 0.002 | | | | | | | | | | |

MORE ↓

| ENTER Enclosed space floor thickness, $L_{crack}$ (cm) | ENTER Soil-bldg. pressure differential, $\Delta P$ ($g/cm\text{-}s^2$) | ENTER Enclosed space floor length, $L_B$ (cm) | ENTER Enclosed space floor width, $W_B$ (cm) | ENTER Enclosed space height, $H_B$ (cm) | ENTER Floor-wall seam crack width, w (cm) | ENTER Indoor air exchange rate, ER (1/h) | ENTER Average vapor flow rate into bldg. OR Leave blank to calculate $Q_{soil}$ (L/m) |
|---|---|---|---|---|---|---|---|
| 10 | 40 | 1000 | 1000 | 244 | 0.1 | 0.25 | |

| ENTER Averaging time for carcinogens, $AT_C$ (yrs) | ENTER Averaging time for noncarcinogens, $AT_{NC}$ (yrs) | ENTER Exposure duration, ED (yrs) | ENTER Exposure frequency, EF (days/yr) | ENTER Target risk for carcinogens, TR (unitless) | ENTER Target hazard quotient for noncarcinogens, THQ (unitless) |
|---|---|---|---|---|---|
| 70 | 30 | 30 | 350 | 1.0E-05 | 1 |

Used to calculate risk-based soil concentration.

END

CHEMICAL PROPERTIES SHEET

| Diffusivity in air, $D_a$ ($cm^2/s$) | Diffusivity in water, $D_w$ ($cm^2/s$) | Henry's law constant at reference temperature, H (atm-$m^3$/mol) | Henry's law constant reference temperature, $T_R$ ($^oC$) | Enthalpy of vaporization at the normal boiling point, $\Delta H_{v,b}$ (cal/mol) | Normal boiling point, $T_B$ ($^oK$) | Critical temperature, $T_C$ ($^oK$) | Organic carbon partition coefficient, $K_{oc}$ ($cm^3/g$) | Pure component water solubility, S (mg/L) | Unit risk factor, URF ($\mu g/m^3)^{-1}$ | Reference conc., RfC ($mg/m^3$) | Physical state at soil temperature, (S,L,G) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 5.65E-02 | 8.02E-06 | 1.19E-02 | 25 | 8,980 | 442.10 | 1220.00 | 7.71E+02 | 2.95E+01 | 0.0E+00 | 3.0E-02 | L |

**END**

INTERMEDIATE CALCULATIONS SHEET

| Exposure duration, $\tau$ (sec) | Source-building separation, $L_T$ (cm) | Stratum A soil air-filled porosity, $\theta_a^A$ ($cm^3/cm^3$) | Stratum B soil air-filled porosity, $\theta_a^B$ ($cm^3/cm^3$) | Stratum C soil air-filled porosity, $\theta_a^C$ ($cm^3/cm^3$) | Stratum A effective total fluid saturation, $S_{te}$ ($cm^3/cm^3$) | Stratum A soil intrinsic permeability, $k_i$ ($cm^2$) | Stratum A soil relative air permeability, $k_{rg}$ ($cm^2$) | Stratum A soil effective vapor permeability, $k_v$ ($cm^2$) | Floor-wall seam perimeter, $X_{crack}$ (cm) | Initial soil concentration used, $C_R$ ($\mu g/kg$) | Bldg. ventilation rate, $Q_{building}$ ($cm^3/s$) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9.46E+08 | 595 | 0.394 | ERROR | ERROR | #N/A | #N/A | #N/A | 1.00E-08 | 4,000 | 1.00E+00 | 1.69E+04 |

| Area of enclosed space below grade, $A_B$ ($cm^2$) | Crack-to-total area ratio, $\eta$ (unitless) | Crack depth below grade, $Z_{crack}$ (cm) | Enthalpy of vaporization at ave. soil temperature, $\Delta H_{v,TS}$ (cal/mol) | Henry's law constant at ave. soil temperature, $H_{TS}$ (atm-$m^3$/mol) | Henry's law constant at ave. soil temperature, $H'_{TS}$ (unitless) | Vapor viscosity at ave. soil temperature, $\mu_{TS}$ (g/cm-s) | Stratum A effective diffusion coefficient, $D^{eff}_A$ ($cm^2/s$) | Stratum B effective diffusion coefficient, $D^{eff}_B$ ($cm^2/s$) | Stratum C effective diffusion coefficient, $D^{eff}_C$ ($cm^2/s$) | Total overall effective diffusion coefficient, $D^{eff}_T$ ($cm^2/s$) | Diffusion path length, $L_d$ (cm) | Convection path length, $L_p$ (cm) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.06E+06 | 3.77E-04 | 15 | 9,495 | 5.08E-03 | 2.19E-01 | 1.75E-04 | 1.32E-02 | 0.00E+00 | 0.00E+00 | 1.32E-02 | 595 | 15 |

| Soil-water partition coefficient, $K_d$ ($cm^3/g$) | Source vapor conc., $C_{source}$ ($\mu g/m^3$) | Crack radius, $r_{crack}$ (cm) | Average vapor flow rate into bldg., $Q_{soil}$ ($cm^3/s$) | Crack effective diffusion coefficient, $D^{crack}$ ($cm^2/s$) | Area of crack, $A_{crack}$ ($cm^2$) | Exponent of equivalent foundation Peclet number, $\exp(Pe^f)$ (unitless) | Infinite source indoor attenuation coefficient, $\alpha$ (unitless) | Infinite source bldg. conc., $C_{building}$ ($\mu g/m^3$) | Finite source $\beta$ term (unitless) | Finite source $\psi$ term $(sec)^{-1}$ | Time for source depletion, $\tau_D$ (sec) | Exposure duration > time for source depletion (YES/NO) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.54E+00 | 1.35E+02 | 0.10 | 1.00E+01 | 1.32E-02 | 4.00E+02 | 1.88E+08 | NA | NA | 3.34E+00 | 3.04E-09 | 5.57E+07 | YES |

| Finite source indoor attenuation coefficient, $<\alpha>$ (unitless) | Mass limit bldg. conc., $C_{building}$ ($\mu g/m^3$) | Finite source bldg. conc., $C_{building}$ ($\mu g/m^3$) | Final finite source bldg. conc., $C_{building}$ ($\mu g/m^3$) | Unit risk factor, URF $(\mu g/m^3)^{-1}$ | Reference conc., RfC ($mg/m^3$) |
|---|---|---|---|---|---|
| NA | 3.27E-03 | NA | 3.27E-03 | NA | 3.0E-02 |

**END**

RESULTS SHEET

RISK-BASED SOIL CONCENTRATION CALCULATIONS:

| Indoor exposure soil conc., carcinogen (µg/kg) | Indoor exposure soil conc., noncarcinogen (µg/kg) | Risk-based indoor exposure soil conc., (µg/kg) | Soil saturation conc., $C_{sat}$ (µg/kg) | Final indoor exposure soil conc., (µg/kg) |
|---|---|---|---|---|
| NA | 9.56E+03 | 9.56E+03 | 4.78E+04 | 9.56E+03 |

INCREMENTAL RISK CALCULATIONS:

| Incremental risk from vapor intrusion to indoor air, carcinogen (unitless) | Hazard quotient from vapor intrusion to indoor air, noncarcinogen (unitless) |
|---|---|
| NA | NA |

MESSAGE AND ERROR SUMMARY BELOW: (DO NOT USE RESULTS IF ERRORS ARE PRESENT)
MESSAGE: The values of Csource and Cbuilding on the INTERCALCS worksheet are based on unity and do not represent actual values.
MESSAGE: Risk/HQ or risk-based soil concentration is based on a route-to-route extrapolation.

**SCROLL DOWN TO "END"**

**END**

Soil Properties Lookup Table

| SCS Soil Type | $K_s$ (cm/h) | $\alpha_1$ (1/cm) | N (unitless) | M (unitless) | n ($cm^3/cm^3$) | $\theta_r$ ($cm^3/cm^3$) | Mean Grain Diameter (cm) | Bulk Density ($g/cm^3$) | $\theta_w$ ($cm^3/cm^3$) | SCS Soil Name |
|---|---|---|---|---|---|---|---|---|---|---|
| C | 0.61 | 0.01496 | 1.253 | 0.2019 | 0.459 | 0.098 | 0.0092 | 1.43 | 0.215 | Clay |
| CL | 0.34 | 0.01581 | 1.416 | 0.2938 | 0.442 | 0.079 | 0.016 | 1.48 | 0.168 | Clay Loam |
| L | 0.50 | 0.01112 | 1.472 | 0.3207 | 0.399 | 0.061 | 0.020 | 1.59 | 0.148 | Loam |
| LS | 4.38 | 0.03475 | 1.746 | 0.4273 | 0.390 | 0.049 | 0.040 | 1.62 | 0.076 | Loamy Sand |
| S | 26.78 | 0.03524 | 3.177 | 0.6852 | 0.375 | 0.053 | 0.044 | 1.66 | 0.054 | Sand |
| SC | 0.47 | 0.03342 | 1.208 | 0.1722 | 0.385 | 0.117 | 0.025 | 1.63 | 0.197 | Sandy Clay |
| SCL | 0.55 | 0.02109 | 1.330 | 0.2481 | 0.384 | 0.063 | 0.029 | 1.63 | 0.146 | Sandy Clay Loam |
| SI | 1.82 | 0.00658 | 1.679 | 0.4044 | 0.489 | 0.050 | 0.0046 | 1.35 | 0.167 | Silt |
| SIC | 0.40 | 0.01622 | 1.321 | 0.2430 | 0.481 | 0.111 | 0.0039 | 1.38 | 0.216 | Silty Clay |
| SICL | 0.46 | 0.00839 | 1.521 | 0.3425 | 0.482 | 0.090 | 0.0056 | 1.37 | 0.198 | Silty Clay Loam |
| SIL | 0.76 | 0.00506 | 1.663 | 0.3987 | 0.439 | 0.065 | 0.011 | 1.49 | 0.180 | Silt Loam |
| SL | 1.60 | 0.02667 | 1.449 | 0.3099 | 0.387 | 0.039 | 0.030 | 1.62 | 0.103 | Sandy Loam |

Chemical Properties Lookup Table

| CAS No. | Chemical | Organic carbon partition coefficient, $K_{oc}$ ($cm^3/g$) | Diffusivity in air, $D_a$ ($cm^2/s$) | Diffusivity in water, $D_w$ ($cm^2/s$) | Pure component water solubility, S (mg/L) | Henry's law constant H' (unitless) | Henry's law constant at reference temperature, H (atm-$m^3$/mol) | Henry's law constant reference temperature, $T_R$ (°C) | Normal boiling point, $T_B$ (°K) | Critical temperature, $T_C$ (°K) | Enthalpy of vaporization at the normal boiling point, $\Delta H_{v,b}$ (cal/mol) | Unit risk factor, URF ($\mu g/m^3)^{-1}$ | Reference conc., RfC ($mg/m^3$) | Physical state at soil temperature, (S,L,G) | URF extrapolated (X) | RfC extrapolated (X) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 56235 | Carbon tetrachloride | 1.74E+02 | 7.80E-02 | 8.80E-06 | 7.93E+02 | 1.24E+00 | 3.03E-02 | 25 | 349.90 | 556.60 | 7,127 | 6.0E-06 | 1.0E-01 | L | | | Surrogate toxicity values (red numbers) used with the surrogate chemical presented below. |
| 57749 | Chlordane | 1.20E+05 | 1.18E-02 | 4.37E-06 | 5.60E-02 | 1.99E-03 | 4.85E-05 | 25 | 624.24 | 885.73 | 14,000 | 1.0E-04 | 7.0E-04 | S | | | |
| 58899 | gamma-HCH (Lindane) | 1.07E+03 | 1.42E-02 | 7.34E-06 | 7.30E+00 | 5.73E-04 | 1.40E-05 | 25 | 596.55 | 839.36 | 15,000 | 3.7E-04 | 1.1E-03 | S | X | X | |
| 60297 | Ethyl ether | 5.73E+00 | 7.82E-02 | 8.61E-06 | 5.68E+04 | 1.35E+00 | 3.29E-02 | 25 | 307.50 | 466.74 | 6,338 | 0.0E+00 | 7.0E-01 | L | | X | |
| 60571 | Dieldrin | 2.14E+04 | 1.25E-02 | 4.74E-06 | 1.95E-01 | 6.18E-04 | 1.51E-05 | 25 | 613.32 | 842.25 | 17,000 | 4.6E-03 | 1.8E-04 | S | | X | |
| 67641 | Acetone | 5.75E-01 | 1.24E-01 | 1.14E-05 | 1.00E+06 | 1.59E-03 | 3.87E-05 | 25 | 329.20 | 508.10 | 6,955 | 0.0E+00 | 3.1E+01 | L | | X | |
| 67663 | Chloroform | 3.98E+01 | 1.04E-01 | 1.00E-05 | 7.92E+03 | 1.50E-01 | 3.66E-03 | 25 | 334.32 | 536.40 | 6,988 | 2.3E-05 | 9.8E-02 | L | | | |
| 67721 | Hexachloroethane | 1.78E+03 | 2.50E-03 | 6.80E-06 | 5.00E+01 | 1.59E-01 | 3.88E-03 | 25 | 458.00 | 695.00 | 9,510 | 1.1E-05 | 3.0E-02 | S | | X | |
| 71432 | Benzene | 5.89E+01 | 8.80E-02 | 9.80E-06 | 1.79E+03 | 2.27E-01 | 5.54E-03 | 25 | 353.24 | 562.16 | 7,342 | 7.8E-06 | 3.0E-02 | L | | | |
| 71556 | 1,1,1-Trichloroethane | 1.10E+02 | 7.80E-02 | 8.80E-06 | 1.33E+03 | 7.03E-01 | 1.72E-02 | 25 | 347.24 | 545.00 | 7,136 | 0.0E+00 | 5.0E+00 | L | | | |
| 72435 | Methoxychlor | 9.77E+04 | 1.56E-02 | 4.46E-06 | 1.00E-01 | 6.46E-04 | 1.58E-05 | 25 | 651.02 | 848.49 | 16,000 | 0.0E+00 | 1.8E-02 | S | | X | |
| 72559 | DDE | 4.47E+06 | 1.44E-02 | 5.87E-06 | 1.20E-01 | 8.59E-04 | 2.09E-05 | 25 | 636.44 | 860.38 | 15,000 | 9.7E-05 | 0.0E+00 | S | X | | |
| 74839 | Methyl bromide | 1.05E+01 | 7.28E-02 | 1.21E-05 | 1.52E+04 | 2.55E-01 | 6.22E-03 | 25 | 276.71 | 467.00 | 5,714 | 0.0E+00 | 5.0E-03 | G | | | |
| 74873 | Methyl chloride (chloromethane) | 2.12E+00 | 1.26E-01 | 6.50E-06 | 5.33E+03 | 3.61E-01 | 8.80E-03 | 25 | 249.00 | 416.25 | 5,115 | 1.8E-06 | 9.0E-02 | L | | | |
| 74908 | Hydrogen cyanide | 3.80E+00 | 1.93E-01 | 2.10E-05 | 1.00E+06 | 5.44E-03 | 1.33E-04 | 25 | 299.00 | 456.70 | 6,676 | 0.0E+00 | 3.0E-03 | L | | | |
| 74953 | Methylene bromide | 1.26E+01 | 4.30E-02 | 8.44E-06 | 1.19E+04 | 3.52E-02 | 8.59E-04 | 25 | 370.00 | 583.00 | 7,868 | 0.0E+00 | 4.0E-04 | L | | X | |
| 75003 | Chloroethane (ethyl chloride) | 4.40E+00 | 2.71E-01 | 1.15E-05 | 5.68E+03 | 3.61E-01 | 8.80E-03 | 25 | 285.30 | 460.40 | 5,879 | 0.0E+00 | 1.0E+01 | L | X | | |
| 75014 | Vinyl chloride (chloroethene) | 1.86E+01 | 1.06E-01 | 1.23E-05 | 8.80E+03 | 1.10E+00 | 2.69E-02 | 25 | 259.25 | 432.00 | 5,250 | 4.4E-06 | 1.0E-01 | G | | | |
| 75058 | Acetonitrile | 4.20E+00 | 1.28E-01 | 1.66E-05 | 1.00E+06 | 1.42E-03 | 3.45E-05 | 25 | 354.60 | 545.50 | 7,110 | 0.0E+00 | 6.0E-02 | L | | | |
| 75070 | Acetaldehyde | 1.06E+00 | 1.24E-01 | 1.41E-05 | 1.00E+06 | 3.23E-03 | 7.87E-05 | 25 | 293.10 | 466.00 | 6,157 | 2.2E-06 | 9.0E-03 | L | | | |
| 75092 | Methylene chloride | 1.17E+01 | 1.01E-01 | 1.17E-05 | 1.30E+04 | 8.96E-02 | 2.18E-03 | 25 | 313.00 | 510.00 | 6,706 | 1.0E-08 | 6.0E-01 | L | | | |
| 75150 | Carbon disulfide | 4.57E+01 | 1.04E-01 | 1.00E-05 | 1.19E+03 | 1.24E+00 | 3.02E-02 | 25 | 319.00 | 552.00 | 6,391 | 0.0E+00 | 7.0E-01 | L | | | |
| 75218 | Ethylene oxide | 1.33E+00 | 1.04E-01 | 1.45E-05 | 3.04E+05 | 2.27E-02 | 5.54E-04 | 25 | 283.60 | 469.00 | 6,104 | 1.0E-04 | 0.0E+00 | L | | | |
| 75252 | Bromoform | 8.71E+01 | 1.49E-02 | 1.03E-05 | 3.10E+03 | 2.41E-02 | 5.88E-04 | 25 | 422.35 | 696.00 | 9,479 | 1.1E-06 | 0.0E+00 | L | | X | |
| 75274 | Bromodichloromethane | 5.50E+01 | 2.98E-02 | 1.06E-05 | 6.74E+03 | 6.54E-02 | 1.60E-03 | 25 | 363.15 | 585.85 | 7,800 | 3.7E-05 | 0.0E+00 | L | X | X | |
| 75296 | 2-Chloropropane | 9.14E+00 | 8.88E-02 | 1.01E-05 | 3.73E+03 | 5.93E-01 | 1.45E-02 | 25 | 308.70 | 485.00 | 6,286 | 0.0E+00 | 1.0E-01 | L | | | |
| 75343 | 1,1-Dichloroethane | 3.16E+01 | 7.42E-02 | 1.05E-05 | 5.06E+03 | 2.30E-01 | 5.61E-03 | 25 | 330.55 | 523.00 | 6,895 | 1.6E-06 | 0.0E+00 | L | | | |
| 75354 | 1,1-Dichloroethylene | 5.89E+01 | 9.00E-02 | 1.04E-05 | 2.25E+03 | 1.07E+00 | 2.60E-02 | 25 | 304.75 | 576.05 | 6,247 | 0.0E+00 | 2.0E-01 | L | | | |
| 75456 | Chlorodifluoromethane | 4.79E+01 | 1.01E-01 | 1.28E-05 | 2.00E+00 | 1.10E+00 | 2.70E-02 | 25 | 232.40 | 369.30 | 4,836 | 0.0E+00 | 5.0E+01 | L | | | |
| 75694 | Trichlorofluoromethane | 4.97E+02 | 8.70E-02 | 9.70E-06 | 1.10E+03 | 3.97E+00 | 9.68E-02 | 25 | 296.70 | 471.00 | 5,999 | 0.0E+00 | 7.0E-01 | L | | | |
| 75718 | Dichlorodifluoromethane | 4.57E+02 | 6.65E-02 | 9.92E-06 | 2.80E+02 | 1.40E+01 | 3.42E-01 | 25 | 243.20 | 384.95 | 9,421 | 0.0E+00 | 1.0E-01 | L | | | |
| 76131 | 1,1,2-Trichloro-1,2,2-trifluoroethar | 1.11E+04 | 7.80E-02 | 8.20E-06 | 1.70E+02 | 1.97E+01 | 4.80E-01 | 25 | 320.70 | 487.30 | 6,463 | 0.0E+00 | 3.0E+01 | L | | | |
| 76448 | Heptachlor | 1.41E+06 | 1.12E-02 | 5.69E-06 | 1.80E-01 | 6.05E+01 | 1.48E+00 | 25 | 603.69 | 846.31 | 13,000 | 1.3E-03 | 1.8E-03 | S | | X | |
| 77474 | Hexachlorocyclopentadiene | 2.00E+05 | 1.61E-02 | 7.21E-06 | 1.80E+00 | 1.10E+00 | 2.69E-02 | 25 | 512.15 | 746.00 | 10,931 | 0.0E+00 | 2.0E-04 | L | | | |
| 78831 | Isobutanol | 2.59E+00 | 8.60E-02 | 9.30E-06 | 8.50E+04 | 4.83E-04 | 1.18E-05 | 25 | 381.04 | 547.78 | 10,936 | 0.0E+00 | 1.1E+00 | L | | X | |
| 78875 | 1,2-Dichloropropane | 4.37E+01 | 7.82E-02 | 8.73E-06 | 2.80E+03 | 1.15E-01 | 2.79E-03 | 25 | 369.52 | 572.00 | 7,590 | 1.0E-05 | 4.0E-03 | L | X | | |
| 78933 | Methylethylketone (2-butanone) | 2.30E+00 | 8.08E-02 | 9.80E-06 | 2.23E+05 | 2.29E-03 | 5.58E-05 | 25 | 352.50 | 536.78 | 7,481 | 0.0E+00 | 5.0E+00 | L | | | |
| 79005 | 1,1,2-Trichloroethane | 5.01E+01 | 7.80E-02 | 8.80E-06 | 4.42E+03 | 3.73E-02 | 9.11E-04 | 25 | 386.15 | 602.00 | 8,322 | 1.6E-05 | 2.0E-04 | L | | X | |
| 79016 | Trichloroethylene | 1.66E+02 | 7.90E-02 | 9.10E-06 | 1.47E+03 | 4.21E-01 | 1.03E-02 | 25 | 360.36 | 544.20 | 7,505 | 4.1E-06 | 3.0E-03 | L | X | | |
| 79209 | Methyl acetate | 3.26E+00 | 1.04E-01 | 1.00E-05 | 2.00E+03 | 4.84E-03 | 1.18E-04 | 25 | 329.80 | 506.70 | 7,260 | 0.0E+00 | 3.5E+00 | L | | X | |
| 79345 | 1,1,2,2-Tetrachloroethane | 9.33E+01 | 7.10E-02 | 7.90E-06 | 2.96E+03 | 1.41E-02 | 3.44E-04 | 25 | 419.60 | 661.15 | 8,996 | 5.8E-05 | 0.0E+00 | L | | X | |
| 79469 | 2-Nitropropane | 1.17E+01 | 9.23E-02 | 1.01E-05 | 1.70E+04 | 5.03E-03 | 1.23E-04 | 25 | 393.20 | 594.00 | 8,383 | 2.7E-03 | 2.0E-02 | L | | | |
| 80626 | Methylmethacrylate | 6.98E+00 | 7.70E-02 | 8.60E-06 | 1.50E+04 | 1.38E-02 | 3.36E-04 | 25 | 373.50 | 567.00 | 8,975 | 0.0E+00 | 7.0E-01 | L | | | |
| 83329 | Acenaphthene | 7.08E+03 | 4.21E-02 | 7.69E-06 | 3.57E+00 | 6.34E-03 | 1.55E-04 | 25 | 550.54 | 803.15 | 12,155 | 0.0E+00 | 0.0E+00 | S | | X | |
| 86737 | Fluorene | 1.38E+04 | 3.63E-02 | 7.88E-06 | 1.98E+00 | 2.60E-03 | 6.34E-05 | 25 | 570.44 | 870.00 | 12,666 | 0.0E+00 | 0.0E+00 | S | | X | |
| 87683 | Hexachloro-1,3-butadiene | 5.37E+04 | 5.61E-02 | 6.16E-06 | 3.20E+00 | 3.33E-01 | 8.13E-03 | 25 | 486.15 | 738.00 | 10,206 | 2.2E-05 | 0.0E+00 | L | | X | |
| 88722 | o-Nitrotoluene | 3.24E+02 | 5.87E-02 | 8.67E-06 | 6.50E+02 | 5.11E-04 | 1.25E-05 | 25 | 495.00 | 720.00 | 12,239 | 0.0E+00 | 0.0E+00 | L | | X | |
| 91203 | Naphthalene | 2.00E+03 | 5.90E-02 | 7.50E-06 | 3.10E+01 | 1.98E-02 | 4.82E-04 | 25 | 491.14 | 748.40 | 10,373 | 3.4E-05 | 3.0E-03 | S | | | |
| 91576 | 2-Methylnaphthalene | 2.81E+03 | 5.22E-02 | 7.75E-06 | 2.46E+01 | 2.12E-02 | 5.17E-04 | 25 | 514.26 | 761.00 | 12,600 | 0.0E+00 | 3.0E-03 | S | | X | Naphthalene |
| 92524 | Biphenyl | 4.38E+03 | 4.04E-02 | 8.15E-06 | 7.45E+00 | 1.23E-02 | 2.99E-04 | 25 | 529.10 | 789.00 | 10,890 | 0.0E+00 | 1.8E-01 | S | | X | |
| 95476 | o-Xylene | 3.63E+02 | 8.70E-02 | 1.00E-05 | 1.78E+02 | 2.12E-01 | 5.18E-03 | 25 | 417.60 | 630.30 | 8,661 | 0.0E+00 | 1.0E-01 | L | | | |
| 95501 | 1,2-Dichlorobenzene | 6.17E+02 | 6.90E-02 | 7.90E-06 | 1.56E+02 | 7.77E-02 | 1.90E-03 | 25 | 453.57 | 705.00 | 9,700 | 0.0E+00 | 2.0E-01 | L | | | |
| 95578 | 2-Chlorophenol | 3.88E+02 | 5.01E-02 | 9.46E-06 | 2.20E+04 | 1.60E-02 | 1.18E+05 | 25 | 447.53 | 675.00 | 9,572 | 0.0E+00 | 2.0E-01 | L | | X | Phenol |
| 95636 | 1,2,4-Trimethylbenzene | 1.35E+03 | 6.06E-02 | 7.92E-06 | 5.70E+01 | 2.52E-01 | 6.14E-03 | 25 | 442.30 | 649.17 | 9,369 | 0.0E+00 | 7.0E-03 | L | | | |
| 96184 | 1,2,3-Trichloropropane | 2.20E+01 | 7.10E-02 | 7.90E-06 | 1.75E+03 | 1.67E-02 | 4.08E-04 | 25 | 430.00 | 652.00 | 9,171 | 0.0E+00 | 3.0E-04 | L | X | | |
| 96333 | Methyl acrylate | 4.53E+00 | 9.76E-02 | 1.02E-05 | 6.00E+04 | 7.68E-03 | 1.87E-04 | 25 | 353.70 | 536.00 | 7,749 | 0.0E+00 | 1.1E-01 | L | | X | |
| 97632 | Ethylmethacrylate | 2.95E+01 | 6.53E-02 | 8.37E-06 | 3.67E+03 | 3.44E-02 | 8.40E-04 | 25 | 390.00 | 571.00 | 10,957 | 0.0E+00 | 3.2E-01 | L | | X | |
| 98066 | tert-Butylbenzene | 7.71E+02 | 5.65E-02 | 8.02E-06 | 2.95E+01 | 4.87E-01 | 1.19E-02 | 25 | 442.10 | 1220.00 | 8,980 | 0.0E+00 | 3.0E-02 | L | | X | Benzene |
| 98828 | Cumene | 4.89E+02 | 6.50E-02 | 7.10E-06 | 6.13E+01 | 4.74E+01 | 1.46E-02 | 25 | 425.56 | 631.10 | 10,335 | 0.0E+00 | 4.0E-01 | L | | | |
| 98862 | Acetophenone | 5.77E+01 | 6.00E-02 | 8.73E-06 | 6.13E+03 | 4.38E-04 | 1.07E-05 | 25 | 475.00 | 709.50 | 11,732 | 0.0E+00 | 3.5E-01 | S,L | | X | |
| 98953 | Nitrobenzene | 6.46E+01 | 7.60E-02 | 8.60E-06 | 2.09E+03 | 9.82E-04 | 2.39E-05 | 25 | 483.95 | 719.00 | 10,566 | 4.0E-05 | 9.0E-03 | L | | | |
| 100414 | Ethylbenzene | 3.63E+02 | 7.50E-02 | 7.80E-06 | 1.69E+02 | 3.22E-01 | 7.86E-03 | 25 | 409.34 | 617.20 | 8,501 | 2.5E-06 | 1.0E+00 | L | | | |
| 100425 | Styrene | 7.76E+02 | 7.10E-02 | 8.00E-06 | 3.10E+02 | 1.12E-01 | 2.74E-03 | 25 | 418.31 | 636.00 | 8,737 | 0.0E+00 | 1.0E+00 | L | | | |
| 100447 | Benzylchloride | 6.14E+01 | 7.50E-02 | 7.80E-06 | 5.25E+02 | 1.70E-02 | 4.14E-04 | 25 | 452.00 | 685.00 | 8,773 | 4.9E-05 | 0.0E+00 | L | X | | |
| 100527 | Benzaldehyde | 4.59E+01 | 7.21E-02 | 9.07E-06 | 3.30E+03 | 9.73E-04 | 2.37E-05 | 25 | 452.00 | 695.00 | 11,658 | 0.0E+00 | 3.5E-01 | L | | X | |
| 103651 | n-Propylbenzene | 5.62E+02 | 6.01E-02 | 7.83E-06 | 6.00E+01 | 4.37E-01 | 1.07E-02 | 25 | 432.20 | 630.00 | 9,123 | 0.0E+00 | 1.0E+00 | L | | X | |
| 104518 | n-Butylbenzene | 1.11E+03 | 5.70E-02 | 8.12E-06 | 2.00E+00 | 5.38E-01 | 1.31E-02 | 25 | 456.46 | 660.50 | 9,290 | 0.0E+00 | 3.0E-02 | L | | X | Benzene |
| 106423 | p-Xylene | 3.89E+02 | 7.69E-02 | 8.44E-06 | 1.85E+02 | 3.13E-01 | 7.64E-03 | 25 | 411.52 | 616.20 | 8,525 | 0.0E+00 | 1.0E-01 | L | | | |

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 106467 | 1,4-Dichlorobenzene | 6.17E+02 | 6.90E-02 | 7.90E-06 | 7.90E+01 | 9.82E-02 | 2.39E-03 | 25 | 447.21 | 684.75 | 9,271 | 1.1E-05 | 8.0E-01 | S | | | |
| 106934 | 1,2-Dibromoethane (ethylene dibr | 2.50E+01 | 2.17E-02 | 1.19E-05 | 4.18E+03 | 3.04E-02 | 7.41E-04 | 25 | 404.60 | 583.00 | 8,310 | 6.0E-04 | 9.0E-03 | L | | | |
| 106990 | 1,3-Butadiene | 1.91E+01 | 2.49E-01 | 1.08E-05 | 7.35E+02 | 3.01E+00 | 7.34E-02 | 25 | 268.60 | 425.00 | 5,370 | 3.0E-02 | 2.0E-03 | L | | | |
| 107028 | Acrolein | 2.76E+00 | 1.05E-01 | 1.22E-05 | 2.13E+05 | 4.99E-03 | 1.22E-04 | 25 | 325.60 | 506.00 | 6,731 | 0.0E+00 | 2.0E-05 | L | | | |
| 107062 | 1,2-Dichloroethane | 1.74E+01 | 1.04E-01 | 9.90E-06 | 8.52E+03 | 4.00E-02 | 9.77E-04 | 25 | 356.65 | 561.00 | 7,643 | 2.6E-05 | 7.0E-03 | L | | | |
| 107131 | Acrylonitrile | 5.90E+00 | 1.22E-01 | 1.34E-05 | 7.40E+04 | 4.21E-03 | 1.03E-04 | 25 | 350.30 | 519.00 | 7,786 | 6.8E-05 | 2.0E-03 | L | | | |
| 108054 | Vinyl acetate | 5.25E+00 | 8.50E-02 | 9.20E-06 | 2.00E+04 | 2.09E-02 | 5.10E-04 | 25 | 345.65 | 519.13 | 7,800 | 0.0E+00 | 2.0E-01 | L | | | |
| 108101 | Methylisobutylketone (4-methyl-2- | 9.06E+00 | 7.50E-02 | 7.80E-06 | 1.90E+04 | 5.64E-03 | 1.38E-04 | 25 | 389.50 | 571.00 | 8,243 | 0.0E+00 | 3.0E+00 | L | | | |
| 108383 | m-Xylene | 4.07E+02 | 7.00E-02 | 7.80E-06 | 1.61E+02 | 3.00E-01 | 7.32E-03 | 25 | 412.27 | 617.05 | 8,523 | 0.0E+00 | 1.0E-01 | L | | | |
| 108678 | 1,3,5-Trimethylbenzene | 1.35E+03 | 6.02E-02 | 8.67E-06 | 2.00E+00 | 2.41E-01 | 5.87E-03 | 25 | 437.89 | 637.25 | 9,321 | 0.0E+00 | 7.0E-03 | L | | | 1,2,4-Trimethylbenzene |
| 108872 | Methylcyclohexane | 7.85E+01 | 7.35E-02 | 8.52E-06 | 1.40E+01 | 4.22E+00 | 1.03E-01 | 25 | 373.90 | 572.20 | 7,474 | 0.0E+00 | 3.0E+00 | L | | | |
| 108883 | Toluene | 1.82E+02 | 8.70E-02 | 8.60E-06 | 5.26E+02 | 2.72E-01 | 6.62E-03 | 25 | 383.78 | 591.79 | 7,930 | 0.0E+00 | 5.0E+00 | L | | | |
| 108907 | Chlorobenzene | 2.19E+02 | 7.30E-02 | 8.70E-06 | 4.72E+02 | 1.51E-01 | 3.69E-03 | 25 | 404.87 | 632.40 | 8,410 | 0.0E+00 | 5.0E-02 | L | | | |
| 109693 | 1-Chlorobutane | 1.72E+01 | 8.26E-02 | 1.00E-05 | 1.10E+03 | 6.93E-01 | 1.69E-02 | 25 | 351.60 | 542.00 | 7,263 | 0.0E+00 | 1.4E+00 | L | | X | |
| 110009 | Furan | 1.86E+01 | 1.04E-01 | 1.22E-05 | 1.00E+04 | 2.21E-01 | 5.39E-03 | 25 | 304.60 | 490.20 | 6,477 | 0.0E+00 | 3.5E-03 | L | | X | |
| 110543 | Hexane | 4.34E+01 | 2.00E-01 | 7.77E-06 | 1.24E+01 | 6.82E+01 | 1.66E+00 | 25 | 341.70 | 508.00 | 6,895 | 0.0E+00 | 2.0E-01 | L | | | |
| 111444 | Bis(2-chloroethyl)ether | 1.55E+01 | 6.92E-02 | 7.53E-06 | 1.72E+04 | 7.36E-04 | 1.80E-05 | 25 | 451.15 | 659.79 | 10,803 | 3.3E-04 | 0.0E+00 | L | | | |
| 115297 | Endosulfan | 2.14E+03 | 1.15E-02 | 4.55E-06 | 5.10E-01 | 4.58E-04 | 1.12E-05 | 25 | 674.43 | 942.94 | 14,000 | 0.0E+00 | 2.1E-02 | S | | X | |
| 118741 | Hexachlorobenzene | 5.50E+04 | 5.42E-02 | 5.91E-06 | 5.00E-03 | 5.40E-02 | 1.32E-03 | 25 | 582.55 | 825.00 | 14,447 | 4.6E-04 | 0.0E+00 | S | | X | |
| 120821 | 1,2,4-Trichlorobenzene | 1.78E+03 | 3.00E-02 | 8.23E-06 | 4.88E+01 | 5.81E-02 | 1.42E-03 | 25 | 486.15 | 725.00 | 10,471 | 0.0E+00 | 2.0E-03 | L | | | |
| 123739 | Crotonaldehyde (2-butenal) | 4.82E+00 | 9.56E-02 | 1.07E-05 | 3.69E+04 | 7.99E-04 | 1.95E-05 | 25 | 375.20 | 568.00 | 9 | 5.4E-04 | 0.0E+00 | L | X | | |
| 124481 | Chlorodibromomethane | 6.31E+01 | 1.96E-02 | 1.05E-05 | 2.60E+03 | 3.20E-02 | 7.81E-04 | 25 | 416.14 | 678.20 | 5,900 | 2.7E-05 | 0.0E+00 | L | X | X | |
| 126987 | Methacrylonitrile | 3.58E+01 | 1.12E-01 | 1.32E-05 | 2.54E+04 | 1.01E-02 | 2.46E-04 | 25 | 363.30 | 554.00 | 7,600 | 0.0E+00 | 7.0E-04 | L | | | |
| 126998 | 2-Chloro-1,3-butadiene (chloropre | 6.73E+01 | 8.58E-02 | 1.03E-05 | 2.12E+03 | 4.91E-01 | 1.20E-02 | 25 | 332.40 | 525.00 | 8,075 | 0.0E+00 | 7.0E-03 | L | | | |
| 127184 | Tetrachloroethylene | 1.55E+02 | 7.20E-02 | 8.20E-06 | 2.00E+02 | 7.53E-01 | 1.84E-02 | 25 | 394.40 | 620.20 | 8,288 | 2.6E-07 | 6.0E-04 | L | | | |
| 129000 | Pyrene | 1.05E+05 | 2.72E-02 | 7.24E-06 | 1.35E+00 | 4.50E-04 | 1.10E-05 | 25 | 667.95 | 936 | 14370 | 0.0E+00 | 0.0E+00 | S | | X | |
| 132649 | Dibenzofuran | 5.15E+03 | 2.38E-02 | 6.00E-06 | 3.10E+00 | 5.15E-04 | 1.26E-05 | 25 | 560 | 824 | 66400 | 0.0E+00 | 0.0E+00 | S | | X | |
| 135988 | sec-Butylbenzene | 9.66E+02 | 5.70E-02 | 8.12E-06 | 3.94E+00 | 5.68E-01 | 1.39E-02 | 25 | 446.5 | 679 | 88730 | 0.0E+00 | 3.0E-02 | L | | X | Benzene |
| 141786 | Ethylacetate | 6.44E+00 | 7.32E-02 | 9.70E-06 | 8.03E+04 | 5.64E-03 | 1.38E-04 | 25 | 350.26 | 523.3 | 7633.66 | 0.0E+00 | 3.2E+00 | L | | X | |
| 156592 | cis-1,2-Dichloroethylene | 3.55E+01 | 7.36E-02 | 1.13E-05 | 3.50E+03 | 1.67E-01 | 4.07E-03 | 25 | 333.65 | 544 | 7192 | 0.0E+00 | 6.0E-02 | L | | X | trans-1,2-Dichloroethylene |
| 156605 | trans-1,2-Dichloroethylene | 5.25E+01 | 7.07E-02 | 1.19E-05 | 6.30E+03 | 3.84E-01 | 9.36E-03 | 25 | 320.85 | 516.5 | 6717 | 0.0E+00 | 6.0E-02 | L | | X | |
| 541731 | 1,3-Dichlorobenzene | 1.98E+03 | 6.92E-02 | 7.86E-06 | 1.34E+02 | 1.27E-01 | 3.09E-03 | 25 | 446 | 684 | 9230.18 | 0.0E+00 | 2.0E-01 | L | | X | 1,2-Dichlorobenzene |
| 309002 | Aldrin | 2.45E+06 | 1.32E-02 | 4.86E-06 | 1.70E-02 | 6.95E-03 | 1.70E-04 | 25 | 603.01 | 839.37 | 15000 | 4.9E-03 | 1.1E-04 | S | | X | |
| 319846 | alpha-HCH (alpha-BHC) | 1.23E+03 | 1.42E-02 | 7.34E-06 | 2.00E+00 | 4.34E-04 | 1.06E-05 | 25 | 596.55 | 839.36 | 15000 | 1.8E-03 | 0.0E+00 | S | | | |
| 542756 | 1,3-Dichloropropene | 4.57E+01 | 6.26E-02 | 1.00E-05 | 2.80E+03 | 7.24E-01 | 1.77E-02 | 25 | 381.15 | 587.38 | 7900 | 4.0E-06 | 2.0E-02 | L | | | |
| 630206 | 1,1,1,2-Tetrachloroethane | 1.16E+02 | 7.10E-02 | 7.90E-06 | 1.10E+03 | 9.90E-02 | 2.41E-03 | 25 | 403.5 | 624 | 9768.282525 | 7.4E-06 | 0.0E+00 | L | | X | |
| 1634044 | MTBE | 7.26E+00 | 1.02E-01 | 1.05E-05 | 5.10E+04 | 2.56E-02 | 6.23E-04 | 25 | 328.3 | 497.1 | 6677.66 | 0.0E+00 | 3.0E+00 | L | | | |
| 7439976 | Mercury (elemental) | 5.20E+01 | 3.07E-02 | 6.30E-06 | 2.00E+01 | 4.40E-01 | 1.07E-02 | 25 | 629.88 | 1750 | 14127 | 0.0E+00 | 3.0E-04 | L | | | |
| 591786 | 2-Hexanone | 1.50E+01 | 7.00E-02 | 8.40E-06 | 1.70E+04 | 3.80E-03 | 9.30E-05 | 25 | 400.8 | 587 | 8554 | 0.0E+00 | 3.0E-02 | L | | | |

**Highlighted chemicals do not have inhalation toxicity values or a surrogate.**