# Constituents of potential concern for human health risk assessment of petroleum fuel releases

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**Supplemental information File 1**



**Supplemental information File 2**

***Table S1: Risk Equations***

| | | |
|---|---|---|
| **INHALATION PATHWAYS** | | |
| Non-Cancer Hazard Quotient | $HQ_{max} = C_{max}^{air} \cdot \frac{EF_{child} \cdot ED_{child}}{ATn_{child} \cdot \left(365 \frac{days}{year}\right) \cdot RfC_i}$ | (1) |
| Cancer Risk | $CR_{max} = C_{max}^{air} \cdot \frac{EF_{adult} \cdot ED_{adult} \cdot URF_i \cdot \left(1000 \frac{\mu g}{mg}\right)}{ATc \cdot \left(365 \frac{days}{year}\right)}$ | (2) |
| **WATER INGESTION PATHWAY** | | |
| Non-Cancer Hazard Quotient | $HQ_{max} = C_{max}^{water} \cdot \frac{EF_{child} \cdot ED_{child} \cdot IR_{child}^{water}}{BW_{child} \cdot ATn_{child} \cdot \left(365 \frac{days}{year}\right) \cdot RfD_o}$ | (3) |
| Cancer Risk | $CR_{max} = C_{max}^{water} \cdot \frac{EF_{adult} \cdot ED_{adult} \cdot IR_{adult}^{water} \cdot SF_o}{BW_{adult} \cdot ATc \cdot \left(365 \frac{days}{year}\right)}$ | (4) |
| **SOIL INGESTION PATHWAY** | | |
| Non-Cancer Hazard Quotient | $HQ_{max} = C_{max}^{soil} \cdot \frac{EF_{child} \cdot ED_{child} \cdot IR_{child}^{soil} \cdot \left(\frac{10^{-6} kg}{mg}\right)}{BW_{child} \cdot ATn_{child} \cdot \left(365 \frac{days}{year}\right) \cdot RfD_o}$ | (5) |
| Cancer Risk | $CR_{max} = C_{max}^{soil} \cdot \frac{EF_{adult} \cdot ED_{adult} \cdot IR_{adult}^{soil} \cdot \left(\frac{10^{-6} kg}{mg}\right) \cdot SF_o}{BW_{adult} \cdot ATc \cdot \left(365 \frac{days}{year}\right)}$ | (6) |
| **SOIL DERMAL CONTACT PATHWAY** | | |
| Non-Cancer Hazard Quotient | $HQ_{max} = C_{max}^{soil} \cdot \frac{EF_{child} \cdot ED_{child} \cdot SA_{child} \cdot M_{child} \cdot \frac{ABS_d}{ABS_{GI}} \cdot \left(\frac{10^{-6} kg}{mg}\right)}{BW_{child} \cdot ATn_{child} \cdot \left(365 \frac{days}{year}\right) \cdot RfD_o}$ | (7) |
| Cancer Risk | $CR_{max} = C_{max}^{soil} \cdot \frac{EF_{adult} \cdot ED_{adult} \cdot SA_{adult} \cdot M_{adult} \cdot \frac{ABS_d}{ABS_{GI}} \cdot \left(\frac{10^{-6} kg}{mg}\right) \cdot SF_o}{BW_{child} \cdot ATc \cdot \left(365 \frac{days}{year}\right)}$ | (8) |
| **COMBINED SOIL DIRECT CONTACT (Inhalation + Ingestion +Dermal Contact)** | | |
| Non-Cancer Hazard Quotient | $[HQ_{max}]_{tot} = [HQ_{max}]_{inhal} + [HQ_{max}]_{ingest} + [HQ_{max}]_{dermal}$ | (9) |
| Cancer Risk | $[CR_{max}]_{tot} = [CR_{max}]_{inhal} + [CR_{max}]_{ingest} + [CR_{max}]_{dermal}$ | (10) |

***Table S2: Equations for Upper-End Hypothetical Source and Exposure Point Concentrations***

**NONAQUEOUS PHASE LIQUIDS**

| Max Source Concentration | Exposure Pathway | Exposure Concentration | Natural Attenuation Factor |
|---|---|---|---|
| $C_{max}^{soil\ gas} = X \cdot P_{vap} = H \cdot S_{eff} \cdot \left(\frac{1000\ L}{m^3}\right)$ (11) | Indoor Inhalation of Vapors | $C_{air}^{max} = C_{max}^{soil\ gas} \cdot DF_{esp}$ (12) | $DF_{esp} = \frac{Q_s}{ER \cdot V_{esp}}$ (13) |

**AFFECTED SOILS**

| Max Source Concentration | Exposure Pathway | Exposure Concentration | Natural Attenuation Factor (ASTM, 2010) |
|---|---|---|---|
| $C_{max}^{soil} = MF \cdot \frac{\rho_{fuel}}{\rho_s} \cdot \theta_{as} \cdot \left(10^6 \frac{mg}{kg}\right)$ (14)<br>$C_{sat}^{soil} = S_{eff} \cdot \frac{\theta_{ws} + k_s \cdot \rho_s + H \cdot \theta_{as}}{\rho_s}$ (15) | Outdoor Inhalation of Vapors and Particulates | $C_{max}^{air} = C_{max}^{soil} \cdot PEF + \min\begin{Bmatrix} C_{max}^{soil} \cdot VF_{ss}^{mb} \\ C_{sat}^{soil} \cdot VF_{ss}^{flux} \end{Bmatrix}$ (16) | $VF_{ss}^{flux} = \frac{2 \cdot W \cdot \rho_s}{U_{air} \delta_{air}} \cdot \sqrt{\frac{D_s^{eff} \cdot H}{\pi\tau \cdot (\theta_{WS} + k_s\rho_s + H\theta_{as})}} \times 10^3$ (20)<br>$VF_{ss}^{mb} = \frac{W \cdot \rho_s \cdot d_s}{U_{air} \cdot \delta_{air} \cdot \tau}$ (21) |
| | Indoor Inhalation of Vapors and Particulates | $C_{max}^{air} = \min\begin{Bmatrix} C_{max}^{soil} \cdot VF_{sesp}^{mb} \\ C_{sat}^{soil} \cdot VF_{sesp}^{flux} \end{Bmatrix}$ (17) | $VF_{sesp}^{flux} = \frac{\frac{H \cdot \rho_s}{(\theta_{WS} + k_s\rho_s + H\theta_{as})} \cdot \left[\frac{D_s^{eff}/L_s}{ER \cdot L_B}\right] \cdot e^{\xi}}{e^{\xi} + \left[\frac{D_s^{eff}/L_s}{ER \cdot L_B}\right] + \left[\frac{D_s^{eff}/L_s}{Q_s/A_b}\right] \cdot [e^{\xi} - 1]} \times 10^3$ (22)<br>$VF_{sesp}^{mb} = \frac{\rho_s \cdot d_s}{L_B \cdot ER \cdot \tau} \times 10^3$ (23) |
| | Dermal Contact | $C_{max}^{soil}$ (18) | N/A |
| | Ingestion | $C_{max}^{soil}$ (19) | N/A |

**AFFECTED GROUNDWATER**

| Max Source Concentration | Exposure Pathway | Exposure Concentration | Natural Attenuation Factor (ASTM, 2010) |
|---|---|---|---|
| $C_{max}^{gw} = S_{eff} = X \cdot S_{aq}$ (24) | Outdoor Inhalation of Vapors and Particulates | $C_{max}^{air} = C_{max}^{gw} \cdot VF_{wamb}^{flux}$ (25) | $VF_{wamb}^{flux} = \frac{H}{1 + \left[\frac{U_{air} \cdot \delta_{air} \cdot L_{GW}}{D_{ws}^{eff} \cdot W}\right]} \times 10^3$ (28) |
| | Indoor Inhalation of Vapors and Particulates | $C_{max}^{air} = C_{max}^{gw} \cdot VF_{wesp}^{flux}$ (26) | $VF_{wesp}^{flux} = \frac{H \cdot \left[\frac{D_{ws}^{eff}/L_{GW}}{ER \cdot L_B}\right] \cdot e^{\xi}}{e^{\xi} + \left[\frac{D_s^{eff}/L_{GW}}{ER \cdot L_B}\right] + \left[\frac{D_{ws}^{eff}/L_s}{Q_s/A_b}\right] \cdot [e^{\xi} - 1]} \times 10^3$ (29) |
| | Ingestion | $C_{max}^{gw} = S_{eff}$ (27) | N/A |

*Table 2 (continued): Equations for Upper-End Hypothetical Source and Exposure Point Concentrations*

**SUPPLEMENTAL CALCULATIONS**

| **Soil-Water Partition Factor** | **Effective Diffusivity Coefficients** (ASTM, 2010) | **Connective Air Flow Through Foundation** (ASTM, 2010) |
|---|---|---|
| $k_s = f_{oc} \cdot K_{oc}$ (30) | $D_s^{eff} = D_{air} \cdot \frac{\theta_{as}^{3.33}}{\theta_T^2} + \left[\frac{D_{wat}}{H}\right] \cdot \left[\frac{\theta_{ws}^{3.33}}{\theta_T^2}\right]$ (31)<br>$D_{ws}^{eff} = (h_c + h_v) \cdot \left[\frac{h_c}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}}\right]$ (32)<br>$D_{cap}^{eff} = D_{air} \cdot \frac{\theta_{acap}^{3.33}}{\theta_T^2} + \left[\frac{D_{wat}}{H}\right] \cdot \left[\frac{\theta_{wcap}^{3.33}}{\theta_T^2}\right]$ (33) | $\xi = \frac{Q_s/A_b}{(D_s^{eff}/L_{crack}) \cdot \eta}$ (34) |

Note: See Table 3 for parameter definitions and default input values.

*Table S3: General Input Parameter Definitions and Values*

| Variable | Definition | Units | Default Value (Residential) | Reference |
|---|---|---|---|---|
| **Exposure Factors** | | | | |
| $ABS_d$ | Dermal absorption factor | unitless | CS | Table 5 |
| $ABS_G$ | Gastrointestinal absorption factor | unitless | CS | |
| ATc | Averaging time - carcinogens | yr | 70 | ASTM 2010, USEPA 1997a |
| ATn | Averaging time - non-carcinogens (Adult) | yr | 30 | ASTM 2010, USEPA 1997a |
| | Averaging time - non-carcinogens (Child) | | 6 | USEPA 1997a |
| BW | Body weight (Adult) | kg | 70 | ASTM 2010, USEPA 1997a |
| | Body weight (Child) | | 15 | USEPA 1997a |
| ED | Exposure duration (Adult) | yr | 30 | ASTM 2010, USEPA 1997a |
| | Exposure duration (Child) | | 6 | USEPA 1997a |
| EF | Exposure frequency (Adult) | d/yr | 350 | ASTM 2010, USEPA 1997a |
| | Exposure frequency (Child) | | 350 | USEPA 1997a |
| $IR^{soil}$ | Soil ingestion rate (Adult) | mg/d | 200 | ASTM 2010, USEPA 1997a |
| | Soil ingestion rate (Child) | | 100 | USEPA 1997a |
| $IR^{water}$ | Water Ingestion rate (Adult) | L/d | 2 | ASTM 2010, USEPA 1997a, WHO 2011 |
| | Water ingestion rate (Child) | | 1 | |
| M | Soil to skin adherence factor (Adult) | $mg/cm^2/d$ | 0.5 | ASTM 2010 |
| SA | Exposed skin surface area (Adult) | $cm^2$ | 6840 | USEPA 1997a |
| | Exposed skin surface area (Child) | | 2520 | |
| **Physical Parameters** | | | | |
| ***Fuel Properties*** | | | | |
| $\rho_{fuel}$ | Fuel liquid density | kg/L | FS | Tables 6, 7, 8 |
| MF | Constituent mass fraction in fuel | unitless | CS / FS | |

*Table S3 (continued): General Input Parameter Definitions and Values*

| Variable | Definition | Units | Default Value (Residential) | Reference |
|---|---|---|---|---|
| ***Soil Properties*** | | | | |
| $\rho_s$ | Soil bulk density | kg/L | 1.7 | ASTM 2010 |
| $\theta_{as}$ | Air-filled soil porosity | unitless | 0.26 | |
| $\theta_{acap}$ | Total air-filled porosity in capillary fringe | unitless | $\theta_T+\theta_{wcap}$ = 0.038 | |
| $\theta_T$ | Total soil porosity | unitless | $\theta_{as}+\theta_{ws}$ = 0.38 | |
| $\theta_{ws}$ | Water-filled soil porosity | unitless | 0.12 | |
| $\theta_{wcap}$ | Total water-filled porosity in capillary fringe | unitless | 0.342 | |
| $f_{oc}$ | Fraction organic carbon in soil | mg-carbon/mg-soil | 0.01 | |
| ***Surface/Source Properties*** | | | | |
| $\delta_{air}$ | Ambient air mixing zone height | cm | 200 | ASTM 2010 |
| $\tau$ | Averaging time for surface vapor emission flux (30 yr) | sec | 9.5E+8 | ASTM 2010 |
| $h_c$ | Vadose zone thickness | cm | 295 | ASTM 2010 |
| $h_c$ | Capillary fringe thickness | cm | 5 | ASTM 2010 |
| $L_{GW}$ | Depth to affected groundwater (=$h_c$+$h_v$) | cm | 3 | ASTM 2010 |
| $L_s$ | Depth to affected subsurface soil source | cm | 15 | ASTM 2010, USEPA 2004a |
| $U_{air}$ | Ambient air velocity in mixing zone | cm/s | 225 | ASTM 2010 |
| W | Source width parallel to wind or groundwater flow direction | cm | 4500 | ASTM 2010 |
| ***Building / Enclosed Space*** | | | | |
| $A_b$ | Slab area | $cm^2$ | 700000 | ASTM 2010 |
| $\eta$ | Foundation crack fraction | unitless | Diffusion Driven: 0.01 / Convection Driven: 0.001 | ASTM 2010, USEPA 2004a |
| ER | Enclosed-space air exchange rate (12 air exchanges per day) | 1/s | 2.8E-4 | ASTM 2010, USEPA 2004a |
| $L_B$ | Enclosed space volume/infiltration area ratio | cm | 200 | ASTM 2010, USEPA 2004a |
| $L_{crack}$ | Enclosed space foundation perimeter | cm | 3400 | ASTM 2010 |
| $Q_s$ | Convective airflow through basement foundation (5 L/min = 83 $cm^3$/sec) | $cm^3$/sec | Diffusion Driven: 0 / Convection Driven: 83 | ASTM 2010, USEPA 2004a |
| $V_{esp}$ | Volume of enclosed space | $cm^3$ | 1.4E+8 | USEPA 2004b |

*Table S3 (continued): General Input Parameter Definitions and Values*

| Variable | Definition | Units | Default Value (Residential) | Reference |
|---|---|---|---|---|
| **Chemical Parameters** | | | | |
| $C_{max,}^{soilgas}$ | Soil gas saturation concentration, in equilibrium with saturated pore water (vapor inhalation pathways) | mg/kg | CS / FS : calc | Eqn. 11 |
| $C_{max,}^{soil}$ | Max. soil saturation for direct contact pathways. Soil pores saturated with fuel. | mg/kg | CS / FS : calc | Eqn. 14, Tables 6, 7, 8 |
| $C_{sat,}^{soil}$ | Soil saturation conc. at equilibrium with effective solubility and vapor pressure (vapor inhalation pathways) | mg/kg | CS / FS : calc | Eqn. 15, Tables 6, 7, 8 |
| $D_{air}$ | Diffusion coefficient in air | $cm^2$/sec | CS | Table 4 |
| $D_{wat}$ | Diffusion coefficient in water | $cm^2$/sec | CS | |
| H | Henry's Law coefficient | unitless | CS | |
| $k_s$ | Soil-water partitioning coefficient | $cm^3$-water/g - soil | calc | Eqn. 30 |
| $K_{oc}$ | Water-organic carbon partitioning coefficient | $cm^3$-water/g - soil | CS | Table 4 |
| $RfC_i$ | Inhalation reference concentration (threshold/non-cancer) | $mg/m^3$ | CS | |
| $RfD_o$ | Oral reference dose (or tolerable daily intake; threshold/non-cancer) | mg/kg/d | CS | |
| $S_{aq}$ | Aqueous solubility (pure form) | mg/L | CS | |
| $S_{eff}$ | Effective solubility = $X \cdot S_{aq}$ | unitless | CS / FS : calc | Eqn. 24, Tables 6, 7, 8 |
| $SF_o$ | Oral slope factor (non-threshold/cancer) | $(mg/kg/d)^{-1}$ | CS | Table 4 |
| $URF_i$ | Inhalation unit risk factor (non-threshold/cancer) | $(ug/m^3)^{-1}$ | CS | |
| X | Constituent mole fraction in fuel | unitless | CS / FS | Tables 6, 7, 8 |
| **Natural Attenuation Factors** | | | | |
| PEF | Particulate emission factor | $(mg/m^3$-air)/(mg/kg-soil) | 6.9E-12 | ASTM 2010 |
| $VF_{sesp}$ | Subsurface soil to enclosed space volatilization factor | $(mg/m^3$-air)/(mg/kg-soil) | CS : calc | Eqn. 22 and 23; ASTM 2010 |
| $VF_{ss}$ | Surface soil to ambient air volatilization factor | $(mg/m^3$-air)/(mg/kg-soil) | CS : calc | Eqn. 20 and 21; ASTM 2010 |
| $VF_{wamb}$ | Groundwater to ambient air volatilization factor | $(mg/m^3$-air)/(mg/L-water) | CS : calc | Eqn. 28; ASTM 2010 |
| $VF_{wesp}$ | Groundwater to enclosed space volatilization factor | $(mg/m^3$-air)/(mg/L-water) | CS : calc | Eqn. 29; ASTM 2010 |
| Notes: CS = chemical specific; SS = site specific; FS = fuel specific. | | | | |

***Table S4: Chemical-Specific Physical and Chemical Properties***

| Compound | H<br>**Henry's Law Constant**<br>*(-)* | log(Koc)<br>**Organic Water Partition Coefficient**<br>*(-)* | $S_{aq}$<br>**Aqueous Solubility**<br>*(mg/l)* | $D_{air}$<br>**Diffusion in Air**<br>*($cm^2/s$)* | $D_{wat}$<br>**Diffusion in Water**<br>*($cm^2/s$)* |
|---|---|---|---|---|---|
| **Individual Constituents** | | | | | |
| Acenaphthene | 6.4E-3 | 3.9E+0 | 4.2E+0 | 4.2E-2 | 7.7E-6 |
| Acenaphthylene | 4.7E-3 | 3.6E+0 | 3.9E+0 | 4.4E-2 | 7.5E-6 |
| Anthracene | 2.7E-3 | 4.5E+0 | 4.3E-2 | 3.2E-2 | 7.7E-6 |
| Benz-a-anthracene | 1.4E-4 | 5.6E+0 | 9.4E-3 | 5.1E-2 | 9.0E-6 |
| Benzene | 2.3E-1 | 1.8E+0 | 1.8E+3 | 8.8E-2 | 9.8E-6 |
| Benzo-a-pyrene | 4.6E-5 | 6.0E+0 | 1.6E-3 | 4.3E-2 | 9.0E+0 |
| Benzo-b-fluoranthene | 4.6E-3 | 6.1E+0 | 1.5E-3 | 2.3E-2 | 5.6E-6 |
| Benzo-e-pyrene | 2.4E-5 | 6.6E+0 | 8.6E-4 | 4.1E-2 | 5.5E-6 |
| Benzo-g,h,i-perylene | 1.1E-5 | 5.0E+0 | 2.6E-4 | 4.9E-2 | 5.7E-6 |
| Biphenyl, 1,1- | 1.2E-2 | 3.7E+0 | 7.5E+0 | 5.7E-2 | 6.7E-6 |
| Chrysene | 3.9E-3 | 5.6E+0 | 1.6E-3 | 2.5E-2 | 6.2E-6 |
| Cumene | 6.1E-1 | 3.5E+0 | 5.0E+1 | 6.5E-2 | 7.1E-6 |
| Cyclohexane | 6.7E+0 | 2.9E+0 | 4.2E+1 | 7.8E-2 | 8.4E-6 |
| Dibromoethane, 1,2- (EDB) | 2.7E-2 | 2.4E+0 | 3.9E+3 | 7.3E-2 | 8.3E-6 |
| Dichloroethane, 1,2- (EDC) | 4.8E-2 | 2.2E+0 | 8.6E+3 | 2.9E-2 | 8.1E-6 |
| Diisopropyl ether (DIPE) | 1.6E-1 | 1.8E+0 | 2.7E+3 | 1.0E-1 | 9.9E-6 |
| Ethyl benzene | 3.2E-1 | 2.6E+0 | 1.7E+2 | 5.4E-2 | 6.8E-6 |
| Ethyl tert-butyl ether (ETBE) | 2..4e-2 | 2.4E+0 | 1.2E+4 | 7.5E-2 | 7.8E-6 |
| Fluoranthene | 6.6E-4 | 5.0E+0 | 2.1E-1 | 3.0E-2 | 6.4E-6 |
| Fluorene | 2.6E-3 | 4.1E+0 | 2.0E+0 | 3.6E-2 | 7.9E-6 |
| Heptane, n- | 8.4E+1 | 3.8E+0 | 2.7E+0 | 6.5E-2 | 7.0E-6 |
| Hexane, n- | 4.7E+1 | 2.7E+0 | 1.3E+1 | 2.0E-1 | 7.8E-6 |
| Indeno-1,2,3-cd-pyrene | 6.6E-5 | 6.5E+0 | 2.2E-5 | 1.9E-2 | 5.7E-6 |
| Methyl cyclohexane | 1.6E+1 | 3.3E+0 | 1.0E+1 | 7.0E-2 | 7.6E-6 |
| Methyl naphthalene, 1- | 1.6E-2 | 3.4E+0 | 2.8E+1 | 6.3E-2 | 7.1E-6 |
| Methyl naphthalene, 2- | 1.8E-2 | 3.6E+0 | 2.5E+1 | 6.3E-2 | 7.2E-6 |
| Methyl tert-butyl ether (MTBE) | 2.4E-2 | 1.9E+0 | 5.1E+4 | 7.9E-2 | 9.4E-6 |
| Naphthalene | 2.0E-2 | 3.3E+0 | 3.1E+1 | 5.9E-2 | 7.5E-6 |
| Phenanthrene | 1.7E-3 | 3.9E+0 | 8.3E-1 | 5.8E-2 | 6.7E-6 |
| Pyrene | 4.5E-4 | 5.0E+0 | 1.4E-1 | 2.7E-2 | 7.2E-6 |
| Tert-amyl-methyl ether (TAME) | 5.4E-2 | 2.4E+0 | 2.6E+3 | 7.3E-2 | 8.5E-6 |
| Tert-butyl alcohol (TBA) | 3.7E-4 | 1.6E+0 | 1.0E+6 | 8.8E-2 | 1.0E-5 |

***Table S4 (continued): Chemical-Specific Physical and Chemical Properties***

| Compound | H<br>**Henry's Law Constant**<br>*(-)* | log(Koc)<br>**Organic Water Partition Coefficient**<br>*(-)* | $S_{aq}$<br>**Aqueous Solubility**<br>*(mg/l)* | $D_{air}$<br>**Diffusion in Air**<br>*($cm^2/s$)* | $D_{wat}$<br>**Diffusion in Water**<br>*($cm^2/s$)* |
|---|---|---|---|---|---|
| Toluene | 2.7E-1 | 2.3E+0 | 5.3E+2 | 8.7E-2 | 8.6E-6 |
| Trimethylbenzene, 1,2,4- | 1.8E-1 | 3.0E+0 | 5.7E+1 | 6.2E-2 | 7.3E-6 |
| Trimethylbenzene, 1,3,5- | 2.7E-1 | 3.0E+0 | 5.1E+1 | 6.2E-2 | 7.2E-6 |
| Xylenes (mixed isomers) | 2.2E-1 | 3.2E+0 | 1.8E+2 | 7.1E-2 | 9.3E-6 |
| **Total Petroleum Hydrocarbon (TPH) Fractions** | | | | | |
| TPH - Aliphatic >C05-C06 | 3.2E+1 | 2.9E+0 | 3.6E+1 | 1.0E-1 | 1.0E-5 |
| TPH - Aliphatic >C06-C08 | 5.0E+1 | 3.6E+0 | 5.4E+0 | 1.0E-1 | 1.0E-5 |
| TPH - Aliphatic >C08-C10 | 8.0E+1 | 4.5E+0 | 4.3E-1 | 1.0E-1 | 1.0E-5 |
| TPH - Aliphatic >C10-C12 | 1.2E+2 | 5.4E+0 | 3.4E-2 | 1.0E-1 | 1.0E-5 |
| TPH - Aliphatic >C12-C16 | 5.2E+2 | 6.7E+0 | 7.6E-4 | 1.0E-1 | 1.0E-5 |
| TPH - Aliphatic >C16-C21 | 4.9E+3 | 8.8E+0 | 2.5E-6 | 1.0E-1 | 1.0E-5 |
| TPH - Aromatic >C10-C12 | 1.4E-1 | 3.4E+0 | 1.5E+1 | 1.0E-1 | 1.0E-5 |
| TPH - Aromatic >C12-C16 | 5.3E-2 | 3.7E+0 | 5.8E+0 | 1.0E-1 | 1.0E-5 |
| TPH - Aromatic >C16-C21 | 1.3E-2 | 4.2E+0 | 6.5E-1 | 1.0E-1 | 1.0E-5 |
| TPH - Aromatic >C21-C35 | 6.7E-4 | 5.1E+0 | 6.6E-3 | 1.0E-1 | 1.0E-5 |

***Table S5: Chemical-Specific Toxicological Parameters***

| Compound | $RfD_o$ Oral Reference Dose (mg/kg/d) | ref | $RfC_i$ Inhalation Reference Concentration ($mg/m^3$) | ref | $SF_o$ Oral Slope Factor $(mg/kg/d)^{-1}$ | ref | $URF_i$ Inhalation Unit Risk Factor $(ug/m^3)^{-1}$ | ref | $ABS_d$ Dermal Absorption Factor (-) | ref | $ABS_{GI}$ Gastrointestinal Absorption Factor (-) | ref |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Individual Constituents** | | | | | | | | | | | | |
| Acenaphthene | 6.0E-2 | B | - | - | 2.0E-4 | A | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Acenaphthylene | 5.0E-2 | A | - | - | 2.0E-3 | A | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Anthracene | 3.0E-1 | B | - | - | - | - | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Benz-a-anthracene | 5.0E-3 | A | - | - | 2.0E-2 | A | 8.8E-5 | C | 1.3E-1 | L | 1.0E+0 | L |
| Benzene | 4.0E-3 | B | 3.0E-2 | B | 3.0E-2 | B | 2.2E-6 | B | 0.0E+0 | L | 1.0E+0 | L |
| Benzo-a-pyrene | 5.0E-4 | A | 2.5E-7 | K | 7.3E+0 | B | 8.7E-2 | D | 1.3E-1 | L | 1.0E+0 | L |
| Benzo-b-fluoranthene | 5.0E-3 | A | - | - | 2.0E-2 | A | 8.8E-5 | C | 1.3E-1 | L | 1.0E+0 | L |
| Benzo-e-pyrene | 3.0E-2 | A | - | - | - | - | - | - | 1.3E-1 | L | 8.9E-1 | L |
| Benzo-g,h,i-perylene | 3.0E-2 | A | - | - | - | - | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Biphenyl, 1,1- | 5.0E-2 | B | - | - | - | - | - | - | 1.0E-1 | L | 5.0E-1 | L |
| Chrysene | 5.0E-2 | A | - | - | 2.0E-3 | A | 8.8E-7 | C | 1.3E-1 | L | 1.0E+0 | L |
| Cumene | 1.0E-1 | B | 4.0E-1 | B | - | - | - | - | 0.0E+0 | L | 8.0E-1 | L |
| Cyclohexane | - | - | 6.0E+0 | B | - | - | - | - | 0.0E+0 | L | 8.0E-1 | L |
| Dibromoethane, 1,2- (EDB) | 9.0E-3 | B | 9.0E-3 | B | 2.0E+0 | B | 6.0E-4 | B | 3.0E-2 | L | 1.0E+0 | L |
| Dichloroethane, 1,2- (EDC) | 1.4E-2 | A | 4.8E-2 | A | 9.1E-2 | B | 2.6E-5 | B | 3.0E-2 | L | 1.0E+0 | L |
| Diisopropyl ether (DIPE) | 5.0E-2 | E | 4.0E-1 | E | - | - | - | - | 3.0E-2 | L | 1.0E+0 | L |
| Ethyl benzene | 1.0E-1 | B | 1.0E+0 | B | - | - | - | - | 0.0E+0 | L | 1.0E+0 | L |
| Ethyl tert-butyl ether (ETBE) | 2.5E-1 | I | 3.0E-1 | B | - | - | - | - | 5.0E-2 | L | 1.0E+0 | L |
| Fluoranthene | 4.0E-2 | B | - | - | 2.0E-3 | A | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Fluorene | 4.0E-2 | B | - | - | - | - | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Heptane, n- | 2.0E+0 | F | 7.0E+0 | F | - | - | - | - | 0.0E+0 | L | 8.0E-1 | L |
| Hexane, n- | 6.0E-2 | G | 6.7E-1 | B | - | - | - | - | 0.0E+0 | L | 8.0E-1 | L |
| Indeno-1,2,3-cd-pyrene | 5.0E-3 | A | - | - | 2.0E-2 | A | 8.8E-5 | C | 1.3E-1 | L | 1.1E+1 | L |
| Methyl cyclohexane | - | - | 3.0E+0 | G | - | - | - | - | 0.0E+0 | L | 1.0E+0 | L |
| Methyl naphthalene, 1- | 7.0E-2 | H | - | - | - | - | - | - | 0.0E+0 | L | 1.0E+0 | L |
| Methyl naphthalene, 2- | 4.0E-3 | B | - | - | - | - | - | - | 0.0E+0 | L | 1.0E+0 | L |
| Methyl tert-butyl ether (MTBE) | 3.0E-1 | I | 3.0E+0 | B | - | - | - | - | 5.0E-2 | L | 1.0E+0 | L |
| Naphthalene | 2.0E-2 | B | 3.0E-3 | B | - | - | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Phenanthrene | 4.0E-2 | A | - | - | - | - | - | - | 1.3E-1 | L | 1.0E+0 | L |

***Table S5 (continued): Chemical-Specific Toxicological Parameters***

| Compound | $RfD_o$ Oral Reference Dose | | $RfC_i$ Inhalation Reference Concentration | | $SF_o$ Oral Slope Factor | | $URF_i$ Inhalation Unit Risk Factor | | $ABS_d$ Dermal Absorption Factor | | $ABS_{GI}$ Gastrointestinal Absorption Factor | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | *(mg/kg/d)* | ref | *($mg/m^3$)* | ref | *$(mg/kg/d)^{-1}$* | ref | *$(ug/m^3)^{-1}$* | ref | *(-)* | ref | *(-)* | ref |
| Pyrene | 3.0E-2 | B | - | - | - | - | - | - | 1.3E-1 | L | 1.0E+0 | L |
| Tert-amyl-methyl ether (TAME) | 1.3E-1 | E | 1.9E-1 | E | - | - | - | - | 3.0E-2 | L | 1.0E+0 | L |
| Tert-butyl alcohol (TBA) | 2.2E-1 | E | 6.3E-2 | E | - | - | - | - | 0.0E+0 | L | 1.0E+0 | L |
| Toluene | 8.0E-2 | B | 5.0E+0 | B | - | - | - | - | 0.0E+0 | L | 1.0E+0 | L |
| Trimethylbenzene, 1,2,4- | 4.0E-1 | J | 3.0E+0 | J | - | - | - | - | 0.0E+0 | L | 8.0E-1 | L |
| Trimethylbenzene, 1,3,5- | 4.0E-1 | J | 3.0E+0 | J | - | - | - | - | 0.0E+0 | L | 8.0E-1 | L |
| Xylenes (mixed isomers) | 2.0E-1 | B | 1.0E-1 | B | - | - | - | - | 3.0E-2 | L | 1.0E+0 | L |
| **Total Petroleum Hydrocarbon (TPH) Fractions** | | | | | | | | | | | | |
| TPH - Aliphatic >C05-C06 | 5.0E+0 | F | 1.8E+1 | F | - | - | - | - | 0.0E+0 | F | 8.0E-1 | F |
| TPH - Aliphatic >C06-C08 | 5.0E+0 | F | 1.8E+1 | F | - | - | - | - | 0.0E+0 | F | 1.0E+0 | F |
| TPH - Aliphatic >C08-C10 | 1.0E-1 | F | 1.0E+0 | F | - | - | - | - | 0.0E+0 | F | 1.0E+0 | F |
| TPH - Aliphatic >C10-C12 | 1.0E-1 | F | 1.0E+0 | F | - | - | - | - | 0.0E+0 | F | 1.0E+0 | F |
| TPH - Aliphatic >C12-C16 | 1.0E-1 | F | 1.0E+0 | F | - | - | - | - | 1.0E-1 | F | 1.0E+0 | F |
| TPH - Aliphatic >C16-C21 | 2.0E+0 | F | - | F | - | - | - | - | 1.0E-1 | F | 1.0E+0 | F |
| TPH - Aromatic >C10-C12 | 4.0E-2 | F | 2.0E-1 | F | - | - | - | - | 0.0E+0 | F | 1.0E+0 | F |
| TPH - Aromatic >C12-C16 | 4.0E-2 | F | 2.0E-1 | F | - | - | - | - | 1.0E-1 | F | 1.0E+0 | F |
| TPH - Aromatic >C16-C21 | 3.0E-2 | F | - | F | - | - | - | - | 1.0E-1 | F | 1.0E+0 | F |
| TPH - Aromatic >C21-C35 | 3.0E-2 | F | - | F | - | - | - | - | 1.0E-1 | F | 1.0E+0 | F |

*Reference key:*

| | | | |
|---|---|---|---|
| A Baars et al., 2001. | D Shell Global Solutions, 2004. | G ATSDR, 2012. | J Environment Agency, 2002. |
| B USEPA, 1993. | E TPHCWG, 1997. | H Tiesjema and Baars, 2009. | K USEPA, 2004c |
| C WHO, 2010. | F USEPA, 1997b. | I Firth, 2008. | |

*Table S6: Fuel-Specific Parameters: Gasoline / Petrol*

| ***Liquid Density: 0.72 kg/L*** <br> ***Average Molecular Weight: 100 g/mol*** | | | | | |
|---|---|---|---|---|---|
| **Compound** | MF | X | $S_{eff}$ | $C_{sat}^{soil}$ | $C_{max}^{soil}$ |
| | **Upper-End Mass Fraction†** | **Mole Fraction** | **Effective Solubility** | **Soil Saturation Concentration (Inhalation)** | **Max Soil Concentration (Direct Contact)** |
| | *(-)* | *(-)* | *(mg/l)* | *(mg/kg)* | *(mg/kg)* |
| **Individual Constituents** | | | | | |
| Benzene | 1.9E-2 | 2.4E-2 | 4.3E+1 | 3.0E+1 | 2.1E+3 |
| Cumene | 1.3E-3 | 1.1E-3 | 5.4E-2 | 1.9E+0 | 1.4E+2 |
| Cyclohexane | 3.9E-3 | 4.6E-3 | 2.0E-1 | 1.7E+0 | 4.3E+2 |
| Dibromoethane, 1,2- (EDB) | 4.1E-4 | 2.2E-4 | 8.5E-1 | 2.4E+0 | 4.5E+1 |
| Dichloroethane, 1,2- (EDC) | 4.4E-4 | 4.4E-4 | 3.8E+0 | 6.0E+0 | 4.8E+1 |
| Diisopropyl ether (DIPE) | 1.5E-1 | 1.5E-1 | 3.9E+2 | 2.9E+2 | 1.7E+4 |
| Ethyl benzene | 1.7E-2 | 1.6E-2 | 2.7E+0 | 1.0E+1 | 1.9E+3 |
| Ethyl tert-butyl ether (ETBE) | 1.5E-1 | 1.5E-1 | 1.8E+3 | 4.8E+3 | 1.7E+4 |
| Heptane, n- | 1.1E-2 | 1.1E-2 | 2.9E-2 | 2.4E+0 | 1.2E+3 |
| Hexane, n- | 2.4E-2 | 2.8E-2 | 3.6E-1 | 4.3E+0 | 2.6E+3 |
| Methyl cyclohexane | 5.8E-3 | 5.9E-3 | 6.1E-2 | 1.5E+0 | 6.4E+2 |
| Methyl naphthalene, 1- | 7.0E-4 | 4.9E-4 | 1.4E-2 | 3.2E-1 | 7.7E+1 |
| Methyl naphthalene, 2- | 1.8E-3 | 1.3E-3 | 3.2E-2 | 1.4E+0 | 2.0E+2 |
| Methyl tert-butyl ether (MTBE) | 1.1E-1 | 1.2E-1 | 6.4E+3 | 5.4E+3 | 1.2E+4 |
| Naphthalene | 2.5E-3 | 2.0E-3 | 6.0E-2 | 1.2E+0 | 2.8E+2 |
| Tert-amyl-methyl ether (TAME) | 1.5E-1 | 1.5E-1 | 3.9E+2 | 1.0E+3 | 1.7E+4 |
| Tert-butyl alcohol (TBA) | -- | -- | 5.0E+2 * | 1.4E+3 | 1.4E+3 * |
| Toluene | 8.1E-2 | 8.8E-2 | 4.6E+1 | 8.9E+1 | 8.9E+3 |
| Trimethylbenzene, 1,2,4- | 3.0E-2 | 2.5E-2 | 1.4E+0 | 1.3E+1 | 3.3E+3 |
| Trimethylbenzene, 1,3,5- | 9.8E-3 | 8.2E-3 | 4.2E-1 | 4.3E+0 | 1.1E+3 |
| **Total Petroleum Hydrocarbon Fractions †** | | | | | |
| TPH - Aliphatic >C05-C06 | 2.2E-1 | 2.7E-1 | 9.8E+0 | 1.3E+2 | 2.4E+4 |
| TPH - Aliphatic >C06-C08 | 3.1E-1 | 3.1E-1 | 1.7E+0 | 8.0E+1 | 3.4E+4 |
| TPH - Aliphatic >C08-C10 | 6.8E-2 | 5.2E-2 | 2.2E-2 | 7.4E+0 | 7.5E+3 |
| TPH - Aliphatic >C10-C12 | 3.1E-2 | 1.9E-2 | 6.6E-4 | 1.7E+0 | 3.4E+3 |
| TPH - Aliphatic >C12-C16 | 1.0E-2 | 5.0E-3 | 3.8E-6 | 1.9E-1 | 1.1E+3 |
| TPH - Aliphatic >C16-C21 | 1.0E-2 | 3.7E-3 | 9.3E-9 | 5.8E-2 | 1.1E+3 |
| TPH - Aromatic >C10-C12 | 2.5E-2 | 1.9E-2 | 4.8E-1 | 1.2E+1 | 2.8E+3 |
| TPH - Aromatic >C12-C16 | 1.0E-3 | 6.7E-4 | 3.9E-3 | 1.9E-1 | 1.1E+2 |
| TPH - Aromatic >C16-C21 | 1.0E-3 | 5.3E-4 | 3.4E-4 | 5.4E-2 | 1.1E+2 |
| TPH - Aromatic >C21-C35 | 1.0E-4 | 4.2E-5 | 2.8E-7 | 3.5E-4 | 1.1E+1 |

Notes:

1) † References for upper-end mass fractions: TPHCWG (1998; Table 4) and SGS (2009).

2) See Table2 for equations used to calculate $C_{sat}$ and $C_{max}$.

3) * Reference for TBA: Figure 2A of API, 2005 (maximum observed concentration in groundwater).

*Table S7: Fuel-Specific Parameters: Diesel / Gas oil*

| ***Liquid Density: 0.83 kg/L*** <br> ***Average Molecular Weight: 200 g/mol*** | | | | | |
|---|---|---|---|---|---|
| **Compound** | MF | X | $S_{eff}$ | $C_{sat}^{soil}$ | $C_{max}^{soil}$ |
| | **Upper-End Mass Fraction†** | **Mole Fraction** | **Effective Solubility** | **Soil Saturation Concentration (Inhalation)** | **Max Soil Concentration (Direct Contact)** |
| | *(-)* | *(-)* | *(mg/l)* | *(mg/kg)* | *(mg/kg)* |
| **Individual Constituents** | | | | | |
| Anthracene | 7.5E-5 | 8.4E-5 | 3.7E-8 | 1.1E-5 | 9.5E+0 |
| Benz-a-anthracene | 1.4E-6 | 1.2E-6 | 1.2E-10 | 4.6E-7 | 1.8E-1 |
| Benzene | 8.4E-4 | 2.2E-3 | 3.8E-2 | 2.6E-2 | 1.1E+2 |
| Benzo-a-pyrene | 2.3E-6 | 1.8E-6 | 2.9E-11 | 3.0E-7 | 2.9E-1 |
| Benzo-b-fluoranthene | 7.6E-7 | 6.0E-7 | 9.0E-12 | 1.1E-7 | 9.6E-2 |
| Benzo-e-pyrene | 5.6E-7 | 4.4E-7 | 3.8E-12 | 1.5E-7 | 7.1E-2 |
| Benzo-g,h,i-perylene | 2.1E-7 | 1.5E-7 | 3.9E-13 | 3.7E-10 | 2.6E-2 |
| Biphenyl, 1,1- | 6.3E-4 | 8.2E-4 | 6.1E-5 | 3.1E-3 | 8.0E+1 |
| Chrysene | 2.1E-6 | 1.8E-6 | 2.9E-11 | 1.2E-7 | 2.6E-1 |
| Cumene | 4.7E-5 | 7.8E-5 | 3.9E-3 | 1.4E-1 | 6.0E+0 |
| Ethyl benzene | 1.3E-3 | 2.4E-3 | 4.0E-3 | 1.5E-2 | 1.6E+2 |
| Fluoranthene | 6.6E-5 | 6.5E-5 | 1.3E-7 | 1.4E-4 | 8.3E+0 |
| Fluorene | 9.1E-4 | 1.1E-3 | 2.2E-5 | 3.0E-3 | 1.2E+2 |
| Indeno-1,2,3-cd-pyrene | 3.8E-7 | 2.8E-7 | 6.1E-14 | 2.1E-9 | 4.8E-2 |
| Methyl naphthalene, 1- | 6.5E-3 | 9.2E-3 | 2.6E-3 | 5.9E-2 | 8.3E+2 |
| Methyl naphthalene, 2- | 1.2E-2 | 1.7E-2 | 4.3E-3 | 1.9E-1 | 1.5E+3 |
| Naphthalene | 3.0E-3 | 4.6E-3 | 1.4E-3 | 2.9E-2 | 3.7E+2 |
| Phenanthrene | 1.1E-3 | 1.2E-3 | 1.0E-5 | 7.3E-4 | 1.4E+2 |
| Pyrene | 5.8E-5 | 5.7E-5 | 7.7E-8 | 8.1E-5 | 7.4E+0 |
| Toluene | 2.8E-3 | 6.1E-3 | 3.2E-2 | 6.1E-2 | 3.5E+2 |
| Trimethylbenzene, 1,3,5- | 3.1E-3 | 5.2E-3 | 2.7E-3 | 2.8E-2 | 4.0E+2 |
| Xylenes (mixed isomers) | 3.6E-3 | 6.7E-3 | 1.2E-2 | 1.5E-1 | 4.5E+2 |
| **Total Petroleum Hydrocarbon Fractions †** | | | | | |
| TPH - Aliphatic >C05-C06 | 0.0E+0 | 0.0E+0 | 9.8E+0 | 1.3E+2 | 0.0E+0 |
| TPH - Aliphatic >C06-C08 | 1.1E-3 | 2.2E-3 | 1.7E+0 | 8.0E+1 | 1.4E+2 |
| TPH - Aliphatic >C08-C10 | 1.3E-2 | 2.1E-2 | 2.2E-2 | 7.4E+0 | 1.7E+3 |
| TPH - Aliphatic >C10-C12 | 5.4E-2 | 6.7E-2 | 2.3E-5 | 5.8E-2 | 6.8E+3 |
| TPH - Aliphatic >C12-C16 | 3.1E-1 | 3.1E-1 | 2.3E-6 | 1.2E-1 | 3.9E+4 |
| TPH - Aliphatic >C16-C21 | 4.2E-1 | 3.1E-1 | 7.8E-9 | 4.9E-2 | 5.3E+4 |
| TPH - Aromatic >C10-C12 | 5.3E-2 | 8.2E-2 | 2.0E-2 | 5.1E-1 | 6.7E+3 |
| TPH - Aromatic >C12-C16 | 7.8E-2 | 1.0E-1 | 6.0E-3 | 3.0E-1 | 9.9E+3 |
| TPH - Aromatic >C16-C21 | 2.7E-4 | 2.8E-4 | 1.8E-6 | 2.9E-4 | 3.4E+1 |
| TPH - Aromatic >C21-C35 | 4.3E-6 | 3.6E-6 | 2.4E-10 | 3.0E-7 | 5.4E-1 |

Notes:

1) † References for upper-end mass fractions: TPHCWG (1998; Tables 10 and 11) and Chevron (2007).

2) See Table2 for equations used to calculate $C_{sat}$ and $C_{max}$.

*Table S8: Fuel-Specific Parameters: Kerosene / Jet Fuel*

| ***Liquid Density: 0.80 kg/L*** <br> ***Average Molecular Weight: 170 g/mol*** | | | | | |
|---|---|---|---|---|---|
| **Compound** | MF | X | $S_{eff}$ | $C_{sat}^{soil}$ | $C_{max}^{soil}$ |
| | **Upper-End Mass Fraction†** | **Mole Fraction** | **Effective Solubility** | **Soil Saturation Concentration (Inhalation)** | **Max Soil Concentration (Direct Contact)** |
| | *(-)* | *(-)* | *(mg/l)* | *(mg/kg)* | *(mg/kg)* |
| **Individual Constituents** | | | | | |
| Acenaphthene | 4.7E-5 | 5.2E-5 | 2.2E-6 | 1.6E-4 | 5.8E+0 |
| Acenaphthylene | 4.5E-5 | 5.0E-5 | 2.0E-6 | 7.7E-5 | 5.5E+0 |
| Anthracene | 1.2E-6 | 1.1E-6 | 5.0E-10 | 1.5E-7 | 1.5E-1 |
| Benzene | 5.0E-3 | 1.1E-2 | 1.9E-1 | 1.3E-1 | 6.1E+2 |
| Ethyl benzene | 7.0E-3 | 1.1E-2 | 1.9E-2 | 7.1E-2 | 8.6E+2 |
| Fluoranthene | 8.6E-6 | 7.2E-6 | 1.5E-8 | 1.6E-5 | 1.1E+0 |
| Fluorene | 4.2E-5 | 4.3E-5 | 8.5E-7 | 1.2E-4 | 5.1E+0 |
| Heptane, n- | 7.3E-3 | 1.2E-2 | 3.3E-4 | 2.7E-2 | 8.9E+2 |
| Methyl naphthalene, 1- | 5.4E-3 | 6.5E-3 | 1.8E-3 | 4.2E-2 | 6.6E+2 |
| Methyl naphthalene, 2- | 1.1E-2 | 1.3E-2 | 3.3E-3 | 1.4E-1 | 1.3E+3 |
| Naphthalene | 3.1E-3 | 4.1E-3 | 1.3E-3 | 2.6E-2 | 3.8E+2 |
| Phenanthrene | 5.8E-4 | 5.5E-4 | 4.5E-6 | 3.3E-4 | 7.1E+1 |
| Pyrene | 2.4E-6 | 2.0E-6 | 2.7E-9 | 2.9E-6 | 2.9E-1 |
| Toluene | 1.6E-2 | 3.0E-2 | 1.6E-1 | 3.0E-1 | 2.0E+3 |
| Trimethylbenzene, 1,3,5- | 2.0E-2 | 2.8E-2 | 1.5E-2 | 1.5E-1 | 2.4E+3 |
| Xylenes (mixed isomers) | 2.5E-2 | 4.0E-2 | 7.0E-2 | 8.9E-1 | 3.1E+3 |
| **Total Petroleum Hydrocarbon Fractions †** | | | | | |
| TPH - Aliphatic >C05-C06 | 3.7E-2 | 7.8E-2 | 2.8E-2 | 3.6E-1 | 4.5E+3 |
| TPH - Aliphatic >C06-C08 | 1.6E-1 | 2.7E-1 | 1.5E-2 | 7.0E-1 | 2.0E+4 |
| TPH - Aliphatic >C08-C10 | 2.8E-1 | 3.7E-1 | 1.6E-3 | 5.2E-1 | 3.4E+4 |
| TPH - Aliphatic >C10-C12 | 3.0E-1 | 3.2E-1 | 1.1E-4 | 2.8E-1 | 3.7E+4 |
| TPH - Aliphatic >C12-C16 | 2.5E-1 | 2.1E-1 | 1.6E-6 | 8.1E-2 | 3.1E+4 |
| TPH - Aliphatic >C16-C21 | 3.0E-2 | 1.9E-2 | 4.7E-10 | 3.0E-3 | 3.7E+3 |
| TPH - Aromatic >C10-C12 | 6.0E-2 | 7.8E-2 | 1.9E-2 | 4.9E-1 | 7.3E+3 |
| TPH - Aromatic >C12-C16 | 1.1E-1 | 1.3E-1 | 7.5E-3 | 3.8E-1 | 1.4E+4 |
| TPH - Aromatic >C16-C21 | 5.4E-3 | 4.8E-3 | 3.1E-5 | 5.0E-3 | 6.6E+2 |
| TPH - Aromatic >C21-C35 | 1.0E-4 | 7.1E-5 | 4.7E-9 | 5.9E-6 | 1.2E+1 |

Notes:

1) † References for upper-end mass fractions: TPHCWG (1998; Table 5) and CONCAWE (2007).

2) See Table2 for equations used to calculate $C_{sat}$ and $C_{max}$.

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