1. Appendix X: Methodology for Developing Statewide Health Standard Vapor Intrusion Screening Values

(Appendix to Statewide health standard VI guidance in the *Technical Guidance Manual*)

The Department has calculated vapor intrusion (VI) screening values (SVs) for use with the Statewide health standard. These screening values may be applied to appropriately collected data for indoor air, sub-slab soil gas, near-source soil gas, soil, and groundwater. The methods used to develop the screening values are explained in the following sections.

The screening values for subsurface media are derived using attenuation factors (α). An attenuation factor is the ratio between the contaminant concentration in indoor air and the equilibrium soil gas concentration in the medium ($\alpha \equiv C_{IA}/C_{SG}$).

As there are distinct attenuation factors for residential (α_R) and nonresidential (α_{NR}) structures, the Department carries out separate calculations for screening values that apply to buildings constructed for residential use that have been converted to a purely nonresidential use. These attenuation factors (α_{CR}) are equal to the residential factors under the assumption that vapor flow rates and indoor air exchange rates are comparable to residential structures. The converted residential screening values are derived from the nonresidential indoor air SVs.

The VI SVs are provided in Tables 1–5 of the Statewide health standard VI guidance section (Section II.B.6.). They will be updated periodically using current toxicological parameter values when Ch. 250 MSCs are revised.

1.1. Indoor Air

Indoor air represents the point of exposure for inhalation of volatile chemicals in the vapor intrusion pathway. The point of application for indoor air screening is the basement or lowest occupied level of the building.

Contaminants that pose a risk for vapor intrusion either have a boiling point less than 200°C or a Henry's law constant greater than or equal to 1×10^{-5} atm-m^3/mol and a molecular weight less than 200 g/mol. Certain regulated substances meet these criteria but currently have no inhalation toxicity values; they are listed in Table X-1. The Department has not published VI SVs for most of these chemicals.

In the case of 1,3,5-trimethylbenzene, the Department has chosen 1,2,4-trimethylbenzene as a surrogate for inhalation toxicity. These two substances have similar chemical and toxicological characteristics, and this selection likely results in conservative SVs.

Indoor air screening values (SV_{IA}) are determined from the inhalation risk equations in U.S. EPA (2009). This method is equivalent to that used by EPA for Regional Screening Levels and in the VISL Calculator (U.S. EPA, 2013a, 2013b). SVs for systemic toxicants ($SV_{IA(nc)}$) and carcinogens ($SV_{IA(c)}$) are calculated in units of micrograms per cubic meter (µg/m^3).

For systemic toxicants (non-carcinogens), the indoor air screening value is:

$$SV_{IA(nc)} = \frac{THQ \times RfC_i \times AT_{nc} \times (365\frac{days}{yr}) \times (24\frac{hr}{day})}{ET \times EF \times ED} \times \frac{1000\ \mu g}{mg}$$

For carcinogens, the indoor air screening value is:

$$SV_{IA(c)} = \frac{TR \times AT_c \times (365\frac{days}{yr}) \times (24\frac{hr}{day})}{IUR \times ET \times EF \times ED}$$

For substances classified as mutagens, except for vinyl chloride and trichloroethylene, the residential carcinogenic indoor air screening value is:

$$SV_{IA(c,m,R)} = \frac{TR \times AT_c \times (365\frac{days}{yr}) \times (24\frac{hr}{day})}{IUR \times ET \times EF \times AED}$$

For vinyl chloride, the residential carcinogenic indoor air screening value is:

$$SV_{IA(c,vc,R)} = \frac{TR}{\frac{IUR \times ET \times EF \times ED}{AT_c \times (365\frac{days}{yr}) \times (24\frac{hr}{day})} + IUR}$$

For trichloroethylene, the residential carcinogenic indoor air screening value is:

$$SV_{IA(c,TCE,R)} = \frac{TR \times AT_c \times (365\frac{days}{yr}) \times (24\frac{hr}{day})}{(IUR_k \times AED + IUR_l \times ED) \times ET \times EF}$$

As TCE has a mutagenic mode of action for the kidneys, the residential carcinogenic SV is calculated using distinct IUR values for kidney cancer and non-Hodgkin lymphoma and liver cancer (U.S. EPA, 2011a).

The variables and exposure factors in the above equations are defined in Table X-2. Certain conditions are explained in 25 Pa. Code §250.307(h).

Residential and nonresidential indoor air screening values are defined as the lower of the applicable systemic, carcinogenic, and/or mutagenic values. The toxicity parameters used are from 25 Pa. Code Ch. 250, Appendix A, Table 5A (Table X-5).

Table X-1. Volatile substances without inhalation toxicity data.

Regulated Substance	CAS No.
ACENAPHTHENE	83-32-9
ACENAPHTHYLENE	208-96-8
ACETOPHENONE	98-86-2
AMMONIUM SULFAMATE	7773-06-0
ANTHRACENE	120-12-7
BENZOTRICHLORIDE	98-07-7
BUTYL ALCOHOL, N-	71-36-3

Regulated Substance	CAS No.
BUTYLATE	2008-41-5
BUTYLBENZENE, N-	104-51-8
BUTYLBENZENE, SEC-	135-98-8
BUTYLBENZENE, TERT-	98-06-6
CHLOROACETALDEHYDE	107-20-0
CHLOROBUTANE, 1-	109-69-3
CHLORONAPHTHALENE, 2-	91-58-7
CHLOROPHENOL, 2-	95-57-8
CHLOROTOLUENE, O-	95-49-8
CHLOROTOLUENE, P-	106-43-4
CRESOL, O- (METHYLPHENOL, 2-)	95-48-7
CROTONALDEHYDE	4170-30-3
CROTONALDEHYDE, TRANS-	123-73-9
DICHLOROBENZENE, 1,3-	541-73-1
DICHLOROETHYLENE, CIS-1,2-	156-59-2
DICHLOROPROPIONIC ACID, 2,2- (DALAPON)	75-99-0
DIISOPROPYL METHYLPHOSPHONATE	1445-75-6
DIMETHYL METHYLPHOSPHONATE	756-79-6
DIMETHYLANILINE, N,N-	121-69-7
DITHIANE, 1,4-	505-29-3
ETHYL ACETATE	141-78-6
ETHYL ACRYLATE	140-88-5
ETHYL DIPROPYLTHIOCARBAMATE, S- (EPTC)	759-94-4
ETHYL ETHER	60-29-7
ETHYLENE CHLORHYDRIN	107-07-3
FLUORENE	86-73-7
FURAN	110-00-9
ISOBUTYL ALCOHOL	78-83-1
METHYL ACETATE	79-20-9
METHYLSTYRENE, ALPHA	98-83-9
METOLACHLOR	51218-45-2
MONOCHLOROACETIC ACID	79-11-8
NITROPHENOL, 2-	88-75-5
NITROPHENOL, 4-	100-02-7
PENTACHLOROETHANE	76-01-7
PHENANTHENE	85-01-8
PHENYL MERCAPTAN	108-98-5
PYRIDINE	110-86-1
TRICHLOROACETIC ACID	76-03-9
TRICHLOROPROPANE, 1,1,2-	598-77-6
TRIMETHYLBENZENE, 1,3,5-	108-67-8
TRINITROGLYCEROL (NITROGLYCERIN)	55-63-0

Table X-2. Inhalation risk variables.

Symbol	Term	Residential	Nonresidential
THQ	Target Hazard Quotient, systemic toxicants	1.0	1.0
RfC_i	Inhalation Reference Concentration (mg/m^3)	Table X-5	Table X-5
AT_{nc}	Averaging Time for systemic toxicants (yr)	30	25
ET	Exposure Time (hr/day)	24	8
EF	Exposure Frequency (days/yr)	350	250
ED	Exposure Duration (yr)	30	25
TR	Target Risk, carcinogens	1×10^{-5}	1×10^{-5}
IUR	Inhalation Unit Risk ($(\mu g/m^3)^{-1}$)	Table X-5	Table X-5
AT_c	Averaging Time for carcinogens (yr)	70	70
AED	Combined Age-Dependent Adjustment Factor and Exposure Duration (yr)	76	N/A
IUR_k	TCE IUR, residential, kidney cancer ($(\mu g/m^3)^{-1}$)	1.0×10^{-6}	N/A
IUR_l	TCE IUR, residential, non-Hodgkin lymphoma and liver cancer ($(\mu g/m^3)^{-1}$)	3.1×10^{-6}	N/A

1.2. Sub-Slab Soil Gas

The point of application for sub-slab soil gas screening is immediately beneath the slab or basement of a building. In some circumstances samples may be collected from behind basement walls and below intact pavement next to buildings. Sub-slab screening values (SV_{SS}) are defined using attenuation factors from U.S. EPA (2012). These screening values have units of micrograms per cubic meter ($\mu g/m^3$).

EPA derived a sub-slab attenuation factor (α_{SS}) from a statistical evaluation of paired sub-slab and indoor air sampling data at 431 residential buildings at 12 sites. The data was limited to chlorinated VOCs. The empirical attenuation factors are defined as $\alpha_{SS} = C_{IA}/C_{SS}$.

EPA's recommended residential attenuation factor is $\alpha_{SS,R} = 0.026$, the 95th percentile of the screened data. The Department has adopted this attenuation factor for all chemicals, including petroleum hydrocarbons, as a conservative approach. This residential factor also applies to nonresidential buildings that were originally constructed for residential use ($\alpha_{SS,CR}$) or that have mixed residential and commercial uses.

For nonresidential buildings that were constructed purely for nonresidential use (e.g., commercial, industrial, and institutional buildings), the Department adjusts EPA's attenuation factor to account for a higher air exchange rate in such structures. The 10th percentile air exchange rates for residential and commercial buildings are 0.18 and 0.60 air changes per hour, respectively (U.S. EPA, 2011b, Ch. 19). These are very conservative rates, particularly for nonresidential buildings which typically have values exceeding 1 hr^{-1}. The adjusted nonresidential sub-slab attenuation factor is:

$$\alpha_{SS,NR} = (0.026) \times \frac{0.18\ hr^{-1}}{0.60\ hr^{-1}} = 0.0078$$

Sub-slab screening values are calculated directly from the indoor air SVs using the applicable attenuation factor:

$$SV_{SS} = \frac{SV_{IA}}{\alpha_{SS}}$$

This method is equivalent to that in EPA's VISL Calculator (U.S. EPA, 2013b).

1.3. Near-Source Soil Gas

Near-source soil gas samples are collected proximal to the source to minimize the influence of variable effects such as soil moisture, atmospheric conditions, and leakage from the surface that can bias shallow soil gas measurements. For groundwater, the point of application is immediately above the capillary zone throughout the area of the plume. For soil in the vadose zone, the point of application is within or immediately above the contaminated soil. The sample must be obtained at least 5 feet below the surface and at or beneath the bottom of the building foundation. Near-source soil gas screening values (SV_{NS}) are defined using attenuation factors derived from modeling as explained below. These SVs have units of micrograms per cubic meter ($\mu g/m^3$).

The Department estimated a near-source soil gas attenuation factor (α_{NS}) by running numerous Johnson & Ettinger model simulations (Johnson and Ettinger, 1991; U.S. EPA, 2004). The Department utilized EPA's advanced soil model (version 3.1, February 2004) to determine a soil gas source concentration corresponding to each specified indoor air screening value. The simulations encompassed 12 to 16 different chemicals, the full suite of soil types, and water-filled porosities ranging from residual saturation to the EPA default values. The Department made conservative assumptions of a shallow source (5 ft) and a high vapor flow rate (Q_{soil} = 5 L/min). EPA's default building characteristics for a small, slab-on-grade residence were retained. The models had low, 10th percentile values for the air exchange rate (0.18 hr^{-1} residential, 0.60 hr^{-1} nonresidential; U.S. EPA, 2011b, Ch. 19).

The results of this modeling indicated that there is relatively little variability in the soil gas attenuation factor for different conditions. The silt soil type has the highest attenuation factor because of its low residual water content and relatively high air-filled porosity. Representative factors are $\alpha_{NS,R}$ = 0.005 and $\alpha_{NS,NR}$ = 0.001 for residential and nonresidential scenarios. To further assess these values the Department examined the soil gas data in EPA's vapor intrusion database (U.S. EPA, 2012). Of 46 buildings at four sites with paired deep soil gas (>10 ft) and indoor air measurements, only one exceeded the modeled attenuation factor of 0.005. (This exception had a measured attenuation factor of 0.0075.)

Near-source screening values are calculated directly from the indoor air values using the applicable attenuation factor:

$$SV_{NS} = \frac{SV_{IA}}{\alpha_{NS}}$$

1.4. Soil

Soil samples may be collected as part of the site characterization or a demonstration of attainment. The point of application is throughout the area of contamination. Screening may be applied when soil contamination is at least 5 feet deep and not in contact with the building

foundation. There must be at least a 5 ft vertical section of clean soil-like material between the contamination and the foundation. Pure-phase contaminants (such as LNAPL) must not be present. Soil screening values (SV_{soil}) are defined as the higher of a calculated screening value and the Department's generic soil-to-groundwater pathway numeric value for a used aquifer. Soil screening values have units of milligrams per kilogram (mg/kg).

The calculated screening value is based on equilibrium partitioning of the contaminant between the sorbed phase on soil, the dissolved phase in pore water, and the vapor phase in the pore space. This relationship is given in 25 Pa. Code §250.308(a)(3), with the dilution factor set to 1:

$$SV'_{soil} = \left(f_{oc}K_{oc} + \frac{\theta_w}{\rho_b}\right) C_{pw} \times \frac{1\ mg}{1000\ \mu g}$$

where SV'_{soil} is the calculated screening value for soil (mg/kg) and C_{pw} is the concentration in pore water (µg/L). The other parameters are defined in Table X-3. The value of f_{oc} is from 25 Pa. Code §250.308(a)(3). The dry bulk density used is representative of typical soil types (U.S. EPA, 2004). The Department defines θ_w equal to 0.1 to represent relatively dry conditions, close to residual saturation, beneath a building.

The pore water concentration is related to the pore vapor concentration (C_{pv}) by Henry's law:

$$C_{pw} = \frac{C_{pv}}{H'} \times \frac{1\ m^3}{1000\ L}$$

where C_{pv} has units of micrograms per cubic meter (µg/m^3). H' is calculated at a soil temperature of 11°C.

The allowable pore vapor concentration is determined from the indoor air screening value by means of attenuation factors equal to the near-source soil gas attenuation factors ($\alpha_{soil} = \alpha_{NS}$):

$$C_{pv} = \frac{SV_{IA}}{\alpha_{soil}}$$

The near-source soil gas attenuation factors were determined through Johnson & Ettinger model testing as described above.

Each calculated screening value is compared to the generic soil-to-groundwater pathway numeric value for a used aquifer (25 Pa. Code Ch. 250, Appendix A, Table 3B), and the higher of the two values is defined as the soil screening value for vapor intrusion (SV_{soil}). The generic soil-to-groundwater numeric values are considered appropriate for vapor intrusion screening because soil contamination that is unable to impact aquifers in excess of groundwater MSCs is also unlikely to pose an excess inhalation risk. The Department also recognizes that these screening values do not account for the natural biological degradation of petroleum hydrocarbons in soil vapor and that soil contamination commonly occurs outside the footprint of potentially impacted buildings.

Table X-3. Soil partitioning parameters.

Symbol	Description	Value
f_{oc}	fraction organic carbon in soil	0.0025
K_{oc}	organic carbon partitioning coefficient (L/kg)	Table X-5
θ_w	water-filled porosity of soil	0.1
ρ_b	dry bulk density of soil (kg/L)	1.5

H'	Henry's law constant at soil temperature	Table X-5

1.5. Groundwater

Groundwater data that has been collected as part of the site characterization or a demonstration of attainment may be used for vapor intrusion screening. The point of application is the area of the groundwater plume. Groundwater cannot be in contact with the building foundation, the depth to water must be at least 5 feet, and there must be at least 5 feet of clean soil-like material between the groundwater and the foundation. Groundwater samples must be collected from properly constructed monitoring wells screened across the water table, and the wetted length of well screen should be no more than 10 feet. Pure-phase contaminants (such as LNAPL) must not be present. Groundwater screening values (SV_{GW}) are defined using attenuation factors from U.S. EPA (2012). Screening values have units of micrograms per liter (µg/L).

EPA derived a groundwater attenuation factor (α_{GW}) from a statistical evaluation of paired groundwater and indoor air sampling data at 774 residential buildings at 24 sites. The data was limited to chlorinated VOCs. The empirical attenuation factors are defined as $\alpha_{GW} = C_{IA}/C_{GW}$.

EPA's recommended residential attenuation factor is 0.0012, the 95th percentile of the screened data. The Department has adopted this attenuation factor for all chemicals, including petroleum hydrocarbons, as a conservative approach. This residential factor ($\alpha_{GW,R}$) also applies to nonresidential buildings that were originally constructed for residential use ($\alpha_{GW,CR}$) or that have mixed residential and commercial use.

For nonresidential buildings that were constructed purely for nonresidential use (e.g., commercial, industrial, and institutional buildings), the Department adjusts EPA's attenuation factor to account for a higher air exchange rate in such structures. The 10th percentile air exchange rates for residential and commercial buildings are 0.18 and 0.60 air changes per hour, respectively (U.S. EPA, 2011b, Ch. 19). The adjusted nonresidential sub-slab attenuation factor is:

$$\alpha_{GW,NR} = (0.0012) \times \frac{0.18\ \text{hr}^{-1}}{0.60\ \text{hr}^{-1}} = 0.00036$$

Calculated groundwater screening values (SV'_{GW}) are determined from the indoor air SVs using the applicable attenuation factor and a conversion from soil gas to a dissolved concentration via Henry's law:

$$SV'_{GW} = \frac{SV_{IA}}{\alpha_{GW}} \times \frac{1}{(1000\ \text{L/m}^3)H'}$$

where H' is the nondimensional Henry's law constant at the groundwater temperature (Table X-5). The Department calculates the Henry's law constant at a groundwater temperature of 11°C.

Each calculated screening value is compared to the groundwater MSC for a used aquifer (25 Pa. Code Ch. 250, Appendix A, Table 1). The groundwater screening value for vapor intrusion (SV_{GW}) is defined as the maximum of the calculated screening value (SV'_{GW}), the MSC, and the aqueous solubility (S). The Department regards the groundwater MSCs as suitable for vapor intrusion screening because they are acceptable for water used inside homes, including inhalation exposures.

1.6. Summary

The attenuation factors used to calculate the vapor intrusion screening values are listed in Table X-4. The sub-slab and groundwater attenuation factors are based on EPA's empirical database (U.S. EPA, 2012). The near-source soil gas and soil attenuation factors are equivalent, and they are defined from the Department's modeling studies.

Table X-4. Attenuation factors

Environmental Medium	α_R	α_{NR}	α_{CR}
Sub-slab soil gas	0.026	0.0078	0.026
Near-source soil gas	0.005	0.001	0.005
Soil	0.005	0.001	0.005
Groundwater	0.0012	0.00036	0.0012

R: residential buildings
NR: nonresidential buildings
CR: residential building converted to nonresidential use

These attenuation factors may also be used within a site-specific standard risk assessment to estimate indoor air concentrations from soil, groundwater, and soil gas data.

1.7. References

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Table X-5. Vapor intrusion screening value calculation parameters.

Regulated Substance	CAS No.	MW (g/mol)	K_{oc} (L/kg)	S (mg/L)	T_B (°C)	T_C (K)	$\Delta H_{v,b}$ (cal/mol)	H (atm-m^3/mol)	H' (@ T_{gw})	RfC_i (mg/m^3)	IUR (µg/m^3)$^{-1}$
ACETALDEHYDE	75-07-0	44.05	4.1	1,000,000	20	466	6,157	6.7×10^{-5}	1.6×10^{-3}	9.0×10^{-3}	2.2×10^{-6}
ACETONE	67-64-1	58.08	0.31	1,000,000	56	508	6,955	3.5×10^{-5}	7.6×10^{-4}	$3.1 \times 10^{+1}$	
ACETONITRILE	75-05-8	41.05	0.5	1,000,000	82	546	7,110	3.5×10^{-5}	7.3×10^{-4}	6.0×10^{-2}	
ACROLEIN	107–2-8	56.06	0.56	208,000	53	506	6,731	1.2×10^{-4}	2.7×10^{-3}	2.0×10^{-5}	
ACRYLAMIDE	79–6-1	71.08	25	2,151,000	193	818	12,363	1.7×10^{-9}	2.2×10^{-8}	6.0×10^{-3}	1.0×10^{-4}
ACRYLIC ACID	79-10-7	72.06	29	1,000,000	141	617	11,000	3.7×10^{-7}	5.0×10^{-6}	1.0×10^{-3}	
ACRYLONITRILE	107-13-1	53.06	11	73,500	77	519	7,786	1.4×10^{-4}	2.7×10^{-3}	2.0×10^{-3}	6.8×10^{-5}
ALLYL ALCOHOL	107-18-6	58.08	3.2	1,000,000	97	545	9,550	5.0×10^{-6}	8.1×10^{-5}	1.0×10^{-4}	
AMMONIA	7664-41-7	17.03	3.1	310,000	–33	406	5,572	1.6×10^{-5}	4.3×10^{-4}	1.0×10^{-1}	
ANILINE	62-53-3	93.13	190	33,800	184	699	10,000	2.0×10^{-6}	3.0×10^{-5}	1.0×10^{-3}	1.6×10^{-6}
BENZENE	71-43-2	78.11	58	1,781	81	562	7,342	5.6×10^{-3}	1.2×10^{-1}	3.0×10^{-2}	7.8×10^{-6}
BENZYL CHLORIDE	100-44-7	126.59	190	493	179	685	8,773	4.1×10^{-4}	6.9×10^{-3}	1.0×10^{-3}	4.9×10^{-5}
BETA PROPIOLACTONE	57-57-8	72.06	4	370,000	162	686	10,285	1.3×10^{-5}	$1.9 \times 10^{+2}$		4.0×10^{-3}
BIPHENYL, 1,1-	92-52-4	154.21	1700	7	255	789	10,890	3.1×10^{-4}	3.9×10^{-3}	4.0×10^{-4}	
BIS(2-CHLOROETHYL)ETHER	111-44-4	143.01	76	10,200	179	660	10,803	1.7×10^{-5}	2.2×10^{-4}		3.3×10^{-4}
BIS(2-CHLORO-ISOPROPYL)ETHER	108-60-1	171.07	62	1,700	189	690	9,695	7.4×10^{-5}	1.1×10^{-3}		1.0×10^{-5}
BIS(CHLOROMETHYL)ETHER	542-88-1	114.96	16	22,000	105	569	7,981	4.4×10^{-3}	8.2×10^{-2}		6.2×10^{-2}
BROMOCHLOROMETHANE	74-97-5	129.38	27	16,700	68	512	7,168	1.5×10^{-3}	3.1×10^{-2}	4.0×10^{-2}	
BROMODICHLOROMETHANE	75-27-4	163.83	93	4,500	87	586	7,800	2.1×10^{-3}	4.2×10^{-2}		3.7×10^{-5}
BROMOMETHANE	74-83-9	94.94	170	17,500	4	467	5,714	7.3×10^{-3}	1.9×10^{-1}	5.0×10^{-3}	
BUTADIENE, 1,3-	106-99–	54.09	120	735	–5	425	5,370	7.4×10^{-2}	$2.0 \times 10^{+0}$	2.0×10^{-3}	3.0×10^{-5}
CARBON DISULFIDE	75-15–	76.13	300	2,100	46	552	6,391	1.4×10^{-2}	3.4×10^{-1}	7.0×10^{-1}	
CARBON TETRACHLORIDE	56-23-5	153.82	160	795	77	557	7,127	2.8×10^{-2}	5.9×10^{-1}	1.0×10^{-1}	6.0×10^{-6}
CHLORO-1,1-DIFLUOROETHANE, 1-	75-68-3	100.5	22	1,400	–9	410	53,298	5.9×10^{-2}	3.6×10^{-2}	$5.0 \times 10^{+1}$	
CHLORO-1-PROPENE, 3- (ALLYL CHLORIDE)	107–5-1	76.53	48	3,300	45	514	6,936	1.1×10^{-2}	2.4×10^{-1}	1.0×10^{-3}	6.0×10^{-6}
CHLOROBENZENE	108-90-7	112.56	200	490	132	632	8,410	3.1×10^{-3}	5.6×10^{-2}	5.0×10^{-2}	
CHLORODIBROMOMETHANE	124-48-1	208.28	83	4,200	116	678	5,900	7.8×10^{-4}	1.9×10^{-2}		2.7×10^{-5}
CHLORODIFLUOROMETHANE	75-45-6	86.47	59	2,899	–41	369	4,836	4.1×10^{-2}	$1.2 \times 10^{+0}$	$5.0 \times 10^{+1}$	

Regulated Substance	CAS No.	MW (g/mol)	K_{oc} (L/kg)	S (mg/L)	T_B (°C)	T_C (K)	$\Delta H_{v,b}$ (cal/mol)	H (atm-m^3/mol)	H' (@ T_{gw})	RfC_i (mg/m^3)	IUR (µg/m^3)$^{-1}$
CHLOROETHANE	75–0-3	64.52	42	5,700	12	460	5,879	1.1×10^{-2}	2.8×10^{-1}	$1.0 \times 10^{+1}$	
CHLOROFORM	67-66-3	119.38	56	8,000	61	536	6,988	3.7×10^{-3}	8.0×10^{-2}	9.8×10^{-2}	2.3×10^{-5}
CHLOROPRENE	126-99-8	88.54	50	1,736	59	525	8,075	5.6×10^{-2}	$1.1 \times 10^{+0}$	2.0×10^{-2}	3.0×10^{-3}
CHLOROPROPANE, 2-	75-29-6	78.54	260	3,100	47	485	6,286	1.8×10^{-2}	4.1×10^{-1}	1.0×10^{-1}	
CRESOL(S)	1319-77-3	108.14	25	20,000	139	701	10,886	1.2×10^{-6}	1.8×10^{-5}	6.0×10^{-1}	
CUMENE (ISOPROPYL BENZENE)	98-82-8	120.2	2800	50	152	631	10,335	1.2×10^{-2}	1.6×10^{-1}	4.0×10^{-1}	
CYCLOHEXANE	110-82-7	84.16	479	55	81	553	7,154	1.5×10^{-1}	$3.2 \times 10^{+0}$	$6.0 \times 10^{+0}$	
CYCLOHEXANONE	108-94-1	98.15	66	36,500	157	653	9,500	9.0×10^{-6}	1.4×10^{-4}	7.0×10^{-1}	
DIBROMO-3-CHLOROPROPANE, 1,2-	96-12-8	236.33	140	1,000	196	704	9,960	1.5×10^{-4}	2.1×10^{-3}	2.0×10^{-4}	6.0×10^{-3}
DIBROMOETHANE, 1,2- (ETHYLENE DIBROMIDE)	106-93-4	187.86	54	4,150	131	583	8,310	6.5×10^{-4}	1.1×10^{-2}	9.0×10^{-3}	6.0×10^{-4}
DIBROMOMETHANE	74-95-3	173.84	110	11,400	96	583	7,868	8.2×10^{-4}	1.6×10^{-2}	4.0×10^{-3}	
DICHLORO-2-BUTENE, 1,4-	764-41–	125	180	850	156	647	8,875	6.6×10^{-4}	1.1×10^{-2}		4.2×10^{-3}
DICHLORO-2-BUTENE, TRANS-1,4-	110-57-6	125	215	850	155	646	9,125	6.6×10^{-4}	1.1×10^{-2}		4.2×10^{-3}
DICHLOROBENZENE, 1,2-	95-50-1	147	350	147	180	705	9,700	1.9×10^{-3}	3.0×10^{-2}	2.0×10^{-1}	
DICHLOROBENZENE, P-	106-46-7	147	510	83	174	685	9,271	2.4×10^{-3}	3.9×10^{-2}	8.0×10^{-1}	1.1×10^{-5}
DICHLORODIFLUOROMETHANE (FREON 12)	75-71-8	120.91	360	280	–30	385	9,421	3.4×10^{-1}	$7.0 \times 10^{+0}$	1.0×10^{-1}	
DICHLOROETHANE, 1,1-	75-34-3	98.96	52	5,000	57	523	6,895	5.6×10^{-3}	1.2×10^{-1}	5.0×10^{-1}	1.6×10^{-6}
DICHLOROETHANE, 1,2-	107–6-2	98.96	38	8,412	83	561	7,643	1.2×10^{-3}	2.4×10^{-2}	7.0×10^{-3}	2.6×10^{-5}
DICHLOROETHYLENE, 1,1-	75-35-4	96.94	65	2,500	32	576	6,247	2.6×10^{-2}	6.3×10^{-1}	2.0×10^{-1}	
DICHLOROETHYLENE, TRANS-1,2-	156-60-5	96.94	47	6,300	48	517	6,717	4.1×10^{-3}	9.2×10^{-2}	6.0×10^{-2}	
DICHLOROMETHANE (METHYLENE CHLORIDE)	75–9-2	84.93	16	20,000	40	510	6,706	3.3×10^{-3}	7.4×10^{-2}	6.0×10^{-1}	1.0×10^{-8}
DICHLOROPROPANE, 1,2-	78-87-5	112.99	47	2,700	96	572	7,590	2.8×10^{-3}	5.6×10^{-2}	4.0×10^{-3}	1.0×10^{-5}
DICHLOROPROPENE, 1,3-	542-75-6	110.97	27	2,700	108	587	7,900	3.6×10^{-3}	6.8×10^{-2}	2.0×10^{-2}	4.0×10^{-6}
DICYCLOPENTADIENE	77-73-6	132.21	810	40	167	665	2,197	6.3×10^{-2}	$2.0 \times 10^{+0}$	7.0×10^{-3}	
DIOXANE, 1,4-	123-91-1	88.11	7.8	1,000,000	101	587	8,690	4.8×10^{-6}	8.6×10^{-5}	1.1×10^{-1}	7.7×10^{-6}
EPICHLOROHYDRIN	106-89-8	92.53	35	65,800	116	600	10	3.0×10^{-5}	1.2×10^{-3}	1.0×10^{-3}	1.2×10^{-6}
ETHOXYETHANOL, 2- (EGEE)	110-80-5	90.12	12	1,000,000	136	572	9,368	4.7×10^{-7}	7.2×10^{-6}	2.0×10^{-1}	
ETHYL BENZENE	100-41-4	106.17	220	161	136	617	8,501	7.9×10^{-3}	1.4×10^{-1}	$1.0 \times 10^{+0}$	

Regulated Substance	CAS No.	MW (g/mol)	K_{oc} (L/kg)	S (mg/L)	T_B (°C)	T_C (K)	$\Delta H_{v,b}$ (cal/mol)	H (atm-m^3/mol)	H' (@ T_{gw})	RfC_i (mg/m^3)	IUR ($\mu g/m^3)^{-1}$
ETHYL METHACRYLATE	97-63-2	114.15	22	4,636	117	571	10,957	5.7×10^{-4}	7.9×10^{-3}	3.0×10^{-1}	
ETHYLENE GLYCOL	107-21-1	62.07	4.4	1,000,000	198	718	12,550	6.0×10^{-8}	6.8×10^{-7}	4.0×10^{-1}	
FLUOROTRICHLOROMETHANE (FREON 11)	75-69-4	137.37	130	1,090	24	471	5,999	9.7×10^{-2}	$2.4 \times 10^{+0}$	7.0×10^{-1}	
FORMALDEHYDE	50–0–	30.03	3.6	55,000	–21	408	5,500	3.4×10^{-7}	9.0×10^{-6}	9.8×10^{-3}	1.3×10^{-5}
FORMIC ACID	64-18-6	46.03	0.54	1,000,000	101	588	5,240	1.7×10^{-7}	4.2×10^{-6}	3.0×10^{-4}	
FURFURAL	98–1-1	96.09	6.3	91,000	162	670	9,826	3.8×10^{-6}	5.8×10^{-5}	5.0×10^{-2}	
HEXACHLOROETHANE	67-72-1	236.74	2200	50	187	695	9,510	3.9×10^{-3}	6.0×10^{-2}	3.0×10^{-2}	1.0×10^{-5}
HEXANE	110-54-3	86.18	3600	10	69	508	6,895	$1.8 \times 10^{+0}$	$3.9 \times 10^{+1}$	7.0×10^{-1}	
HYDRAZINE/HYDRAZINE SULFATE	302–1-2	32.05	0.0053	1,000,000	114	653	10,700	6.1×10^{-7}	9.3×10^{-6}	3.0×10^{-5}	4.9×10^{-3}
METHACRYLONITRILE	126-98-7	67.09	21	25,700	90	554	7,600	2.5×10^{-4}	4.9×10^{-3}	3.0×10^{-2}	
METHANOL	67-56-1	32.04	2.8	1,000,000	65	513	8,426	4.6×10^{-6}	8.6×10^{-5}	$4.0 \times 10^{+0}$	
METHOXYETHANOL, 2-	109-86-4	76.1	0	1,000,000	124	598	8,966	3.3×10^{-7}	5.6×10^{-6}	2.0×10^{-2}	
METHYL ACRYLATE	96-33-3	86.09	55	52,000	70	536	7,749	2.0×10^{-4}	4.0×10^{-3}	2.0×10^{-2}	
METHYL CHLORIDE	74-87-3	50.49	6	6,180	–24	416	5,115	8.8×10^{-3}	2.4×10^{-1}	9.0×10^{-2}	1.8×10^{-6}
METHYL ETHYL KETONE	78-93-3	72.11	32	275,000	80	537	7,481	5.7×10^{-5}	1.2×10^{-3}	$5.0 \times 10^{+0}$	
METHYL HYDRAZINE	60-34-4		1	1,000,000	88	585	8,890	3.0×10^{-6}	5.4×10^{-5}	2.0×10^{-5}	1.0×10^{-3}
METHYL ISOBUTYL KETONE	108-10-1	100.16	17	19,550	117	571	8,243	1.4×10^{-4}	2.5×10^{-3}	$3.0 \times 10^{+0}$	
METHYL ISOCYANATE	624-83-9	57.05	10	100,000	40	491	6,394	9.3×10^{-4}	2.2×10^{-2}	1.0×10^{-3}	
METHYL METHACRYLATE	80-62-6	100.12	10	15,600	100	567	8,975	3.2×10^{-4}	5.5×10^{-3}	7.0×10^{-1}	
METHYL N-BUTYL KETONE (2-HEXANONE)	591-78-6	100.16	54	17,500	128	601	8,610	9.3×10^{-5}	1.6×10^{-3}	3.0×10^{-2}	
METHYL STYRENE (MIXED ISOMERS)	25013-15-4	118.18	2200	89	163	655	12,027	2.6×10^{-3}	3.1×10^{-2}	4.0×10^{-2}	
METHYL TERT-BUTYL ETHER (MTBE)	1634–4-4	88.15	12	45,000	55	497	6,678	5.9×10^{-4}	1.3×10^{-2}	$3.0 \times 10^{+0}$	2.6×10^{-7}
METHYLNAPHTHALENE, 2-	91-57-6	142.2	16,000	25	241	761	12,600	5.2×10^{-4}	5.5×10^{-3}	3.0×10^{-3}	
NAPHTHALENE	91-20-3	128.18	950	30	218	748	10,373	4.4×10^{-4}	6.1×10^{-3}	3.0×10^{-3}	
NITROBENZENE	98-95-3	123.11	130	2,000	211	719	10,566	2.4×10^{-5}	3.2×10^{-4}	9.0×10^{-3}	4.0×10^{-5}
NITROPROPANE, 2-	79-46-9	89.09	20	16,700	120	594	8,383	1.2×10^{-4}	2.1×10^{-3}	2.0×10^{-2}	2.7×10^{-3}
NITROSODIETHYLAMINE, N-	55-18-5	102.14	26	93,000	176	655	10,087	3.6×10^{-6}	5.2×10^{-5}		4.3×10^{-2}

Regulated Substance	CAS No.	MW (g/mol)	K_{oc} (L/kg)	S (mg/L)	T_B (°C)	T_C (K)	$\Delta H_{v,b}$ (cal/mol)	H (atm-m^3/mol)	H' (@ T_{gw})	RfC_i (mg/m^3)	IUR (µg/m^3)$^{-1}$
NITROSODIMETHYLAMINE, N-	62-75-9	74.08	8.5	1,000,000	154	645	9,448	1.8×10^{-6}	2.9×10^{-5}	4.0×10^{-5}	1.4×10^{-2}
NITROSO-DI-N-BUTYLAMINE, N-	924-16-3	158.25	450	1,200	235	584	11,653	1.3×10^{-5}	9.8×10^{-5}		1.6×10^{-3}
PCB-1221 (AROCLOR)	11104-28-2	188.66	1900	1	275	845	12,100	7.4×10^{-4}	8.5×10^{-3}		5.7×10^{-4}
PCB-1232 (AROCLOR)	11141-16-5	188.66	1500	1	290	845	12,200	7.4×10^{-4}	8.1×10^{-3}		5.7×10^{-4}
PHENOL	108-95-2	94.11	22	84,300	182	694	10,920	3.3×10^{-7}	4.5×10^{-6}	2.0×10^{-1}	
PROPANOL, 2- (ISOPROPYL ALCOHOL)	67-63–	60.1	25	1,000,000	82	508	9,518	8.1×10^{-6}	1.3×10^{-4}	$7.0 \times 10^{+0}$	
PROPYLBENZENE, N-	103-65-1	120.2	720	52	159	630	9,123	1.1×10^{-2}	1.7×10^{-1}	$1.0 \times 10^{+0}$	
PROPYLENE OXIDE	75-56-9	58.08	25	405,000	34	482	6,621	7.0×10^{-5}	1.6×10^{-3}	3.0×10^{-2}	3.7×10^{-6}
STYRENE	100-42-5	104.15	910	300	145	636	8,737	2.8×10^{-3}	4.7×10^{-2}	$1.0 \times 10^{+0}$	
TETRACHLOROETHANE, 1,1,1,2-	630-20-6	167.85	980	1,100	131	624	9,768	2.5×10^{-3}	3.9×10^{-2}		7.4×10^{-6}
TETRACHLOROETHANE, 1,1,2,2-	79-34-5	167.85	79	2,860	147	661	8,996	3.7×10^{-4}	6.2×10^{-3}		5.8×10^{-5}
TETRACHLOROETHYLENE (PCE)	127-18-4	165.83	300	162	121	620	8,288	1.8×10^{-2}	3.3×10^{-1}	4.0×10^{-2}	2.6×10^{-7}
TETRAHYDROFURAN	109-99-9	72.106	43	300,000	66	541	7,074	7.1×10^{-5}	$1.5 \times 10^{+2}$	$2.0 \times 10^{+0}$	1.9×10^{-6}
TOLUENE	108-88-3	92.14	130	532	111	592	7,930	6.6×10^{-3}	1.3×10^{-1}	$5.0 \times 10^{+0}$	
TRIBROMOMETHANE (BROMOFORM)	75-25-2	252.73	130	3,050	149	696	9,479	5.4×10^{-4}	8.9×10^{-3}		1.1×10^{-6}
TRICHLORO-1,2,2-TRIFLUOROETHANE, 1,1,2-	76-13-1	187.38	1200	170	48	487	6,463	5.3×10^{-1}	$1.2 \times 10^{+1}$	$3.0 \times 10^{+1}$	
TRICHLOROBENZENE, 1,2,4-	120-82-1	181.45	1500	44	213	725	10,471	1.4×10^{-3}	1.9×10^{-2}	2.0×10^{-3}	
TRICHLOROBENZENE, 1,3,5-	108-70-3	181.45	3100	6	208	744	10,600	1.9×10^{-3}	2.6×10^{-2}	2.0×10^{-3}	
TRICHLOROETHANE, 1,1,1-	71-55-6	133.41	100	1,495	74	545	7,136	1.7×10^{-2}	3.7×10^{-1}	$5.0 \times 10^{+0}$	
TRICHLOROETHANE, 1,1,2-	79–0-5	133.41	76	4,420	114	602	8,322	8.2×10^{-4}	1.5×10^{-2}	2.0×10^{-4}	1.6×10^{-5}
TRICHLOROETHYLENE (TCE)	79–1-6	131.39	93	1,100	87	544	7,505	9.9×10^{-3}	2.0×10^{-1}	2.0×10^{-3}	4.0×10^{-6}
TRICHLOROPROPANE, 1,2,3-	96-18-4	147.43	280	1,896	157	652	9,171	3.4×10^{-4}	5.6×10^{-3}	3.0×10^{-4}	
TRICHLOROPROPENE, 1,2,3-	96-19-5	145.42	190	2,700	142	623	8,585	1.8×10^{-2}	3.0×10^{-1}	3.0×10^{-4}	
TRIETHYLAMINE	121-44-8	101.19	51	55,000	90	536	8,095	1.5×10^{-4}	2.8×10^{-3}	7.0×10^{-3}	
TRIMETHYLBENZENE, 1,3,4- (TRIMETHYLBENZENE, 1,2,4-)	95-63-6	120.2	2200	56	169	649	9,369	6.2×10^{-3}	9.5×10^{-2}	7.0×10^{-3}	
TRIMETHYLBENZENE, 1,3,5- *	108-67-8	120.2	660	49	165	637	9,321	8.8×10^{-3}	1.4×10^{-1}	7.0×10^{-3}	
VINYL ACETATE	108–5-4	86.09	2.8	20,000	73	519	7,800	5.1×10^{-4}	1.0×10^{-2}	2.0×10^{-1}	

Regulated Substance	CAS No.	MW (g/mol)	K_{oc} (L/kg)	S (mg/L)	T_B (°C)	T_C (K)	$\Delta H_{v,b}$ (cal/mol)	H (atm-m^3/mol)	H' (@ T_{gw})	RfC_i (mg/m^3)	IUR (µg/m^3)$^{-1}$
VINYL BROMIDE (BROMOETHENE)	593-60-2	106.95	150	4,180	16	464	5,398	1.2×10^{-2}	3.2×10^{-1}	3.0×10^{-3}	3.2×10^{-5}
VINYL CHLORIDE	75–1-4	62.5	10	2,700	–13	432	5,250	2.8×10^{-2}	7.5×10^{-1}	1.0×10^{-1}	9.0×10^{-6}
XYLENES (TOTAL)	1330-20-7	106.17	350	175	140	616	8,523	5.2×10^{-3}	9.0×10^{-2}	1.0×10^{-1}	

Notes to Table X-5.

*** 1,3,5-trimethylbenzene does not have a RfC_i value defined in Title 25 Pa. Code Ch. 250, Appendix A, Table 5A. The Department has selected 1,2,4-trimethylbenzene as a surrogate chemical and assigns its RfC_i as a conservative value.**

Symbol	Definition	Source
MW	molecular weight	VISL Calculator (U.S. EPA, 2013b), or alternate
K_{oc}	organic carbon partition coefficient	Title 25 Pa. Code Ch. 250, Appendix A, Table 5A
S	aqueous solubility	Title 25 Pa. Code Ch. 250, Appendix A, Table 5A
T_B	boiling point temperature	Title 25 Pa. Code Ch. 250, Appendix A, Table 5A
T_C	critical temperature	VISL Calculator (U.S. EPA, 2013b), or alternate
$\Delta H_{v,b}$	enthalpy of vaporization at the normal boiling point	VISL Calculator (U.S. EPA, 2013b), or alternate
H	Henry's law constant	VISL Calculator (U.S. EPA, 2013b), or alternate
H'	Dimensionless Henry's law constant	Calculated using formula in the VISL Calculator (U.S. EPA, 2013b)
RfC_i	Inhalation reference concentration	Title 25 Pa. Code Ch. 250, Appendix A, Table 5A
IUR	Inhalation unit risk	Title 25 Pa. Code Ch. 250, Appendix A, Table 5A

Alternate sources include:

- The U.S. National Institutes of Health online Hazardous Substances Data Bank (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB)
- DEP's Land Recycling Program online Chemical and Physical Properties Database (http://www.depreportingservices.state.pa.us/ReportServer/Pages/ReportViewer.aspx?/CPP/Chemicals)
- EPA's Johnson & Ettinger model (U.S. EPA, 2004)