

S-Risk for the Walloon region - substance datasheet:

N-hexane-2025

1,1-Dichloroéthylène-2025

1,2,4-Triméthylbenzène-2025

1,3,5-Triméthylbenzène-2025

1,2,3-Triméthylbenzène-2025

2,4,5-Trichlorophénol-2025

2,4,6-Trichlorophénol-2025

Warning message:

**The data contained in the current BD PNN database (v8)
have not yet been updated**

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List of acronyms

ABS	Absorption factor
Al	Aluminum content
BCF	Bioconcentration factor
BTF	Biotransfer factor
Da	Diffusion coefficient in air
Dpe	Diffusion coefficient in polyethylene
Dpvc	Diffusion coefficient in PVC
Dw	Diffusion coefficient in water
FA	Factor used when calculating dermal absorption from water
Fe	Iron content
ISSeP	Institut Scientifique de Service Public
K _d	Sorption coefficient soil-water
Koa	Distribution coefficient octanol-air
Koc	Distribution coefficient organic carbon-water
Kow	Distribution coefficient octanol-water
Kp	Dermale permeability coefficient
PAH	polycyclic aromatic hydrocarbons
Ptot	Total phosphorus content
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document

N-hexane-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	N-hexane	Pubchem
Name S-Risk WAL	-	N-hexane-2025	
Molecular formula		C ₆ H ₁₄	Pubchem
CAS number	-	110-54-3	Pubchem
EC number	-	203-777-6 295-570-2	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	Ssi 2 < pKa < 12 (pKa =14,2)
Molar mass – M	g/mol	86,175	Lide (2009-2010)
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	9,5	Mcauliffe (1966) in SRC PHYSPROP database (March 2017)
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	2,017E+04	Boublik et al (1984) in SRC PHYSPROP database (March 2017)
Temperature for Henry coefficient - Th	°C	10	
Henry coefficient - H	Pa.m ³ /mol	2,412E+04	Ashwoth et al. (1988) in Mackay et al. (2006)
Organic carbon-water partition coefficient - Koc	dm ³ /kg	132	USEPA calculated value from INERIS (March 2017) / http://www.ineris.fr/substances/fr/substance/1073
Log Koc		2,120	
Octanol-water partition coefficient - Kow	-	7,943E+03	Hansch et al. (1995) in SRC physprop database (March 2017)
Log Kow		3,9	
Permeation organic substance through PE pipe - Dpe	m ² /d	4,000E-06	Lijzen et al.2001 (value for TPH aliph EC5-EC8)

Permeation organic substance through PVC pipe - Dpvc	m ² /d	(4,000E-09)	calculated by S-Risk
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	(1,96.10 ⁻¹)	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
Other root vegetables (such as radish)		Calculation using chemical and plant properties
Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek		Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties
Leafy vegetables		
Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties
Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties

Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)		Use model
Cow liver BTF	(mg/kg fw)/(mg/d)		Use model
Cow kidney BTF	(mg/kg fw)/(mg/d)		Use model
Cow milk BTF	(mg/kg fw)/(mg/d)		Use model
Sheep meat BTF	(mg/kg fw)/(mg/d)		Use model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)	0	

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	7.10 ⁻¹	US-EPA IRIS (2005)
TDI oral	mg/(kg.d)	1.10 ⁻¹	Santé Canada (2021) and US-EPA (2005)
TDI dermal	mg/(kg.d)	1.10 ⁻¹	= TDI oral
Systemic effects non-threshold			

Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$		
Oral slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		
Dermal slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		

1,1-Dichloroethylene-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	1,1-Dichloroethylene	Pubchem
Name S-Risk WAL	-	1,1-Dichloroethylene-2025	
Molecular formula		C ₂ H ₂ Cl ₂	Pubchem
CAS number	-	75-35-4	Pubchem
EC number	-	200-864-0	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	
Molar mass – M	g/mol	96,943	Mackay D. et al. (2006), Syracuse Research Center (SRC) - BD PHYSPROP
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	2,420E+03	Syracuse Research Center (SRC) - BD PHYSPROP and Pubchem (HSDB), EXP - Verschueren K. (1996) proposed 2500 at 25°C
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	7,999E+04	Syracuse Research Center (SRC) - BD PHYSPROP and Pubchem (HSDB), EXP - Verschueren K. (1996) proposed 66661 (500 mmHg) at 20°C
Temperature for Henry coefficient - Th	°C	10	
Henry coefficient - H	Pa.m ³ /mol	1,560E+03	Mackay D. et al (2006), EXP – worst case of 2 values at 10 °C (1287;1560).

			Pubchem (HSDB) and Syracuse Research Center (SRC) - BD PHYSPROP Proposed 2645 (2,61E-2 atm.m3/mol) at 24°C
Organic carbon-water partition coefficient - Koc	dm ³ /kg	150	Mackay D. et al (2006) calculated from Kow (Kenaga et Goring, 1980)
Log Koc		2,176	
Octanol-water partition coefficient - Kow	-	1,349E+02	Pubchem (HSDB)-Verschuieren K. (1996)- Syracuse Research Center (SRC) - BD PHYSPROP, EXP. Mackay D. et al (2006) also proposed 2,16 (recommended, Sangster et Hansch)
Log Kow		2,130	
Permeation organic substance through PE pipe - Dpe	m ² /d	0	No available data in Lijzen (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d		No data
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	(1,15.10 ⁻²)	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
Other root vegetables (such as radish)		Calculation using chemical and plant properties

Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek		Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties
Leafy vegetables		
Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties
Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties
Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)		Use model
Cow liver BTF	(mg/kg fw)/(mg/d)		Use model
Cow kidney BTF	(mg/kg fw)/(mg/d)		Use model
Cow milk BTF	(mg/kg fw)/(mg/d)		Use model
Sheep meat BTF	(mg/kg fw)/(mg/d)		Use model

Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)	0	

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³	0,07	CQ AWAC
Indoor air	mg/m ³	0,07	CQ AWAC

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	$7 \cdot 10^{-2}$	OEHHA
TDI oral	mg/(kg.d)	$5 \cdot 10^{-2}$	US-EPA
TDI dermal	mg/(kg.d)	$5 \cdot 10^{-2}$	= oral TDI
Systemic effects non-threshold			
Unit risk for inhalation	(mg/m ³) ⁻¹	$5 \cdot 10^{-2}$	US-EPA withdrawn – SPAQuE decision
Oral slope factor	(mg/kg.d) ⁻¹	$6 \cdot 10^{-1}$	US-EPA withdrawn – SPAQuE decision
Dermal slope factor	(mg/kg.d) ⁻¹	$6 \cdot 10^{-1}$	= oral SF

1,2,4-Trimethylbenzene-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	1,2,4-Trimethylbenzene	Pubchem
Name S-Risk WAL	-	1,2,4-Trimethylbenzene-2025	
Molecular formula		C ₉ H ₁₂	Pubchem
CAS number	-	95-63-6	Pubchem
EC number	-	202-436-9	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	
Molar mass – M	g/mol	120,191	Mackay et al. (2006) Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Second Edition. CRC
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	5,700E+01	Mcauliffe (1966) in SRC PHYSPROP database (March 2017)
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	2,800E+02	Chao et al. (1983) in SRC physprop database (March 2017)
Temperature for Henry coefficient - Th	°C	15	
Henry coefficient - H	Pa.m ³ /mol	3,770E+02	Sanemasa et al. (1982) in Mackay et al. (2006)
Organic carbon-water partition coefficient - Koc	dm ³ /kg	1905	Kollig (1995) in Mackay et al. (2006), calculated value
Log Koc		3,280	
Octanol-water partition coefficient - Kow	-	4,266E+03	Hansch et al. (1995) in SRC physprop

			database (march 2017)
Log Kow		3,630	
Permeation organic substance through PE pipe - Dpe	m ² /d	0	No available data in Lijzen (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d		No data
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	$(8,37 \cdot 10^{-2})$	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
Other root vegetables (such as radish)		Calculation using chemical and plant properties
Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek		Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties
Leafy vegetables		
Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties

Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties
Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)		Use model
Cow liver BTF	(mg/kg fw)/(mg/d)		Use model
Cow kidney BTF	(mg/kg fw)/(mg/d)		Use model
Cow milk BTF	(mg/kg fw)/(mg/d)		Use model
Sheep meat BTF	(mg/kg fw)/(mg/d)		Use model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)	0	

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	6.10 ⁻²	US-EPA IRIS (2016)
TDI oral	mg/(kg.d)	1.10 ⁻²	US-EPA IRIS (2016)
TDI dermal	mg/(kg.d)	1.10 ⁻²	= oral TDI

Systemic effects non-threshold			
Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$		
Oral slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		
Dermal slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		

1,3,5-Trimethylbenzene-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	1,3,5-Trimethylbenzene	Pubchem
Name S-Risk WAL	-	1,3,5-Trimethylbenzene-2025	
Molecular formula		C ₉ H ₁₂	Pubchem
CAS number	-	108-67-8	Pubchem
EC number	-	203-604-4	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	
Molar mass – M	g/mol	120,191	Mackay et al. (2006) Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Second Edition. CRC
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	4,820E+01	Yalkowsky and He (2003) in SRC PHYSPROP database (March 2017)
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	3,306E+02	Dauber and Danner (1989) in SRC physprop database (March 2017)
Temperature for Henry coefficient - Th	°C	10	
Henry coefficient - H	Pa.m ³ /mol	4,080E+02	Ashwoth et al. (1988) in Mackay et al. (2006)
Organic carbon-water partition coefficient - Koc	dm ³ /kg	661	Schwarzenbach & Westall (1981) in Mackay et al. (2006)
Log Koc		2,820	
Octanol-water partition coefficient - Kow	-	2,630E+03	Hansch et al. (1995) in SRC physprop

			database (March 2017)
Log Kow		3,420	
Permeation organic substance through PE pipe - Dpe	m ² /d	0	No available data in Lijzen (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d		No data
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	$(6,08 \cdot 10^{-2})$	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
Other root vegetables (such as radish)		Calculation using chemical and plant properties
Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek		Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties
Leafy vegetables		
Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties

Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties
Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)		Use model
Cow liver BTF	(mg/kg fw)/(mg/d)		Use model
Cow kidney BTF	(mg/kg fw)/(mg/d)		Use model
Cow milk BTF	(mg/kg fw)/(mg/d)		Use model
Sheep meat BTF	(mg/kg fw)/(mg/d)		Use model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)	0	

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	6.10 ⁻²	US-EPA IRIS (2016)
TDI oral	mg/(kg.d)	1.10 ⁻²	US-EPA IRIS (2016)
TDI dermal	mg/(kg.d)	1.10 ⁻²	= oral TDI

Systemic effects non-threshold			
Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$		
Oral slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		
Dermal slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		

1,2,3-Trimethylbenzene-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	1,2,3-Trimethylbenzene	Pubchem
Name S-Risk WAL	-	1,2,3-Trimethylbenzene-2025	
Molecular formula		C ₉ H ₁₂	Pubchem
CAS number	-	526-73-8	Pubchem
EC number	-	247-099-9 208-394-8	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	
Molar mass - M	g/mol	120,191	Mackay et al. (2006) Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Second Edition. CRC
Temperature for water solubility - Ts	°C	15	
Water solubility - S	mg/l	7,520E+01	Mackay (measured value selected at the lowest temperature, Sanemasa et al, 1982)
Temperature for P - Tp	°C	16,8	
Vapour pressure - Pa	Pa	1,333E+02	Mackay (value selected at the lowest temperature)
Temperature for Henry coefficient - Th	°C	15	
Henry coefficient - H	Pa.m ³ /mol	2,412E+02	Mackay (measured value selected at the lowest temperature, Sanemasa et al, 1982)
Organic carbon-water partition coefficient - Koc	dm ³ /kg	631	Mackay (mean from 5 soils and 3 sediments proposed by Mackay, Schwarzenbach & Westall, 1981)
Log Koc		2,800	

Octanol-water partition coefficient - Kow	-	4,467E+03	Mackay (geometric mean of 9 values)
Log Kow		3,650	
Permeation organic substance through PE pipe - Dpe	m ² /d	0	No available data in Lijzen (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d		No data
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	$(8,63 \cdot 10^{-2})$	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
Other root vegetables (such as radish)		Calculation using chemical and plant properties
Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek		Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties
Leafy vegetables		
Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties

Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties
Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)		Use model
Cow liver BTF	(mg/kg fw)/(mg/d)		Use model
Cow kidney BTF	(mg/kg fw)/(mg/d)		Use model
Cow milk BTF	(mg/kg fw)/(mg/d)		Use model
Sheep meat BTF	(mg/kg fw)/(mg/d)		Use model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)	0	

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	6.10 ⁻²	US-EPA IRIS (2016)
TDI oral	mg/(kg.d)	1.10 ⁻²	US-EPA IRIS (2016)
TDI dermal	mg/(kg.d)	1.10 ⁻²	= oral TDI

Systemic effects non-threshold			
Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$		
Oral slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		
Dermal slope factor	$(\text{mg}/\text{kg}.\text{d})^{-1}$		

2,4,5-Trichlorophenol-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	2,4,5-Trichlorophenol	Pubchem
Name S-Risk WAL	-	2,4,5-Trichlorophenol-2025	
Molecular formula		C ₆ H ₂ Cl ₃ OH	Pubchem
CAS number	-	95-95-4	Pubchem
EC number	-	202-467-8	Pubchem
Organic	-	Yes	
Dissociating	-	Yes	
Type Acid/Base	-	Acid	
Acid constant - pKa		7,4	Arcand et al. (1985) in SRC physprop database (March 2017)
Molar mass – M	g/mol	197,446	Mackay et al. (2006) Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Second Edition. CRC
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	1,200E+03	Leuenberger et al. (1985 A) in SRC physprop database (March 2017)
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	9,999E-01	Bidleman and Renberg (1985) in SRC physprop database (March 2017)
Temperature for Henry coefficient - Th	°C	8	
Henry coefficient - H	Pa.m ³ /mol	1,320E-01	Leuenberger et al. (1985) in Mackay et al. (2006)
Organic carbon-water partition coefficient - Koc	dm ³ /kg	1877	Mackay et al. (2006), geometric mean of 4

			values
Log Koc		3,270	
Octanol-water partition coefficient - Kow	-	5,248E+03	Hansch et al. (1995) in SRC physprop database (March 2017)
Log Kow		3,720	
Permeation organic substance through PE pipe - Dpe	m ² /d	5,000E-07	Lijzen (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d	(5,000E-10)	Calculated by S-Risk
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	(3,54.10 ⁻²)	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
Other root vegetables (such as radish)		Calculation using chemical and plant properties
Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek		Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties

Leafy vegetables		
Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties
Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties
Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)		Use model
Cow liver BTF	(mg/kg fw)/(mg/d)		Use model
Cow kidney BTF	(mg/kg fw)/(mg/d)		Use model
Cow milk BTF	(mg/kg fw)/(mg/d)		Use model
Sheep meat BTF	(mg/kg fw)/(mg/d)		Use model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)	0	

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	1.10 ⁻²	Route-to-route extrapolation (inhalation pathway not relevant)

TDI oral	mg/(kg.d)	$3 \cdot 10^{-3}$	RIVM (1991) based on 2,4-dichlorophenol
TDI dermal	mg/(kg.d)	$3 \cdot 10^{-3}$	= oral TDI
Systemic effects non-threshold			
Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$		
Oral slope factor	$(\text{mg}/\text{kg.d})^{-1}$		
Dermal slope factor	$(\text{mg}/\text{kg.d})^{-1}$		

2,4,6-Trichlorophenol-2025

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	2,4,6-Trichlorophenol	Pubchem
Name S-Risk WAL	-	2,4,6-Trichlorophenol - 2025	
Molecular formula		C ₆ H ₂ Cl ₃ OH	Pubchem
CAS number	-	88-06-2	Pubchem
EC number	-	201-795-9	Pubchem
Organic	-	Yes	
Dissociating	-	Yes	
Type Acid/Base	-	Acid	
Acid constant - pKa		6,23	Chem IDplus, HSDB, PHYSPROP
Molar mass - M	g/mol	197,446	Mackay et al. (2006) Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Second Edition. CRC
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	8,000E+02	800 mg/L (25, EXP, ChemIDplus, PHYSPROP, INERIS), 500 mg/L (HSBD)
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	1,067E+00	0,008 mmHg (25°, HSBD, PHYSPROP, US-EPA); 1,2 Pa (INERIS)
Temperature for Henry coefficient - Th	°C	20	
Henry coefficient - H	Pa.m ³ /mol	4,280E-01	Sheikheldin et al. (2001) in Mackay et al. (2006)
Organic carbon-water partition coefficient - Koc	dm ³ /kg	1777	150-2200 (HSBD); 380 (US-EPA), 711 et 1777 (INERIS); 1777 (MCI et 1894 (with Kow) calculated with EPIsuite.

Log Koc		3,250	
Octanol-water partition coefficient - Kow	-	4,898E+03	3,69 (chemIDplus, EXP, HSDB, PHYSPROP, US-EPA, INERIS)
Log Kow		3,690	
Permeation organic substance through PE pipe - Dpe	m ² /d	5,000E-07	Lijzen (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d	(5,000E-10)	Calculated by S-Risk
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	0,059	Roberts (1977) in US-EPA- RAGS-E (2004)
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	Default value
Fraction absorbed water - FA	-	1	Default value

Plant	BCF plant	Source
Potatoes		
Potatoes		Calculation using chemical and plant properties
Root and tuber vegetables		
Carrots		Calculation using chemical and plant properties
Salsify		Calculation using chemical and plant properties
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Bulbous vegetables		
Bulbous vegetables (such as onion)		Calculation using chemical and plant properties
Leek	Leek	Calculation using chemical and plant properties
Fruiting vegetables		
Tomato		Calculation using chemical and plant properties
Cucumber		Calculation using chemical and plant properties
Other fruiting vegetables (such as peppers)		Calculation using chemical and plant properties
Cabbages		
Cabbage		Calculation using chemical and plant properties
Cauliflower and broccoli		Calculation using chemical and plant properties
Sprouts		Calculation using chemical and plant properties
Leafy vegetables		

Lettuce		Calculation using chemical and plant properties
Lamb's lettuce		Calculation using chemical and plant properties
Endive		Calculation using chemical and plant properties
Spinach		Calculation using chemical and plant properties
Chicory		Calculation using chemical and plant properties
Celery		Calculation using chemical and plant properties
Legumes		
Beans		Calculation using chemical and plant properties
Peas		Calculation using chemical and plant properties
Grasses		
Grass		Calculation using chemical and plant properties
Cereals		
maize		Calculation using chemical and plant properties

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Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)	0	
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Limit value	Unit	Value	Source
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Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	3,5.10 ⁻³	Route-to-route extrapolation (inhalation pathway not relevant)

TDI oral	mg/(kg.d)	1.10^{-3}	US EPA PPRTV (2007)
TDI dermal	mg/(kg.d)	1.10^{-3}	= oral TDI
Systemic effects non-threshold			
Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$	2.10^{-2}	Route-to-route extrapolation (inhalation pathway not relevant)
Oral slope factor	$(\text{mg}/\text{kg.d})^{-1}$	7.10^{-2}	OEHHA (2009)
Dermal slope factor	$(\text{mg}/\text{kg.d})^{-1}$	7.10^{-2}	= oral SF

References

See annex 1 of the Non-Regulated Pollutants protocol ([link](#)).



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