

Substance data Sheet BDE 99

Parameter	Unit	Value	Source
Name		2,2',4,4',5-Pentabromodiphenyl ether	
CAS number		60348-60-9	
EC number			
Type			
Dissociative			
Acid constant (pKa)		-	BDE-99 does not ionize under environmental conditions (AICIS, 2020)
Molar mass	g/mol	564.7	
Water solubility	mg/l	0.0054 (at 25°C)	Average value experimental data (Tittlemier et al., 2002; Kuramochi et al., 2007; Stenzel and Markley, 1997)
Vapour pressure	Pa	4.3e-5 (at 25°C)	Average value experimental data (Tittlemier et al., 2002; Kuramochi et al., 2007; Wong et al., 2001; EC, 2002)
Henry coefficient	Pa m ³ /mol	1.07 (at 25°C)	
Log K _{ow}	g/g	7.36	
K _{ow}		2.29x10 ⁺⁷	
Log K _{oc}	dm ³ /kg	6,4	Average value experimental data
K _{oc}		2.51x10 ⁺⁶	
Log K _{oa}	g/g		Estimated in S-Risk
BCF	(mg/kg dm)/(mg/m ³)	see table below	
Dpe	m ² /d	1x10 ⁻⁷	Lijzen et al. (2018)
Dpvc	m ² /d	1x10 ⁻¹⁰	Cornelis et al (2017)
Diffusion for organic substance in air (Da)	m ² /d	0.308	Cornelis et al (2022)
Diffusion for organic substance in water (Dw)	m ² /d	3.17x10 ⁻⁵	Cornelis et al (2022)
Kp	[cm/h]	0.0373	DermWin
Fraction absorbed water (FA)	-	1	ATSDR, 2017
ABS dermal soil/dust		0.1	EPA, 2004
RBA soil/dust		0.81	Huwe et al. (2008)
BTF beef	d/kg	1.3x10 ⁻²	Takaki et al. (2015)
BTF sheepmeat	d/kg		Estimated in S-Risk
BTF liver	d/kg	1.2x10 ⁻²	Kierkegaard et al. (2009)
BTF kidney	d/kg		Estimated in S-Risk
BTF milk	d/kg	9x10 ⁻³	Kierkegaard et al. (2009); Takaki et al. (2015)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity	No data available		
Systemic effects threshold			
TDI oral	mg/kg.d	1x10 ⁻⁴	US EPA (2008)
TCA inhalatory	[mg/m ³]	3.5-4	US EPA (2008)

TDI dermal	mg/kg.d	8.5x10 ⁻⁵	US EPA (2008)
smoothing - ages			
Systemic effects non threshold			
Slope factor oral	(mg/kg/d)	Not available	
Unit risk inhalation	(mg/m ³)	Not available	
Slope factor dermal	(mg/kg/d)	Not available	
Limit in air	mg/m ³	3.5x10 ⁻⁴	toxicological reference value
Limit in drinking water	mg/m ³	0.6	SRV for groundwater
Crop standard	mg/kg fw	-	
Meat and edible offal standard		-	
Beef	mg/kg fw	-	
Sheepmeat	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background all age groups including children	mg/kg/d	1.25x10 ⁻⁷ (1 - < 3 y)	Based on concentrations from Poma et al (2018) and food consumption data from S-RISK
	mg/kg/d	9.92x10 ⁻⁸ (3 - < 6 y)	
	mg/kg/d	6.65x10 ⁻⁸ (6 - < 10 y)	
	mg/kg/d	4.04x10 ⁻⁸ (10 - < 15 y)	
	mg/kg/d	2.98 x10 ⁻⁸ (15 - < 21 y)	
	mg/kg/d	2.86 x10 ⁻⁸ (21 - < 31 y)	
	mg/kg/d	2.66 x10 ⁻⁸ (31 - < 41 y)	
	mg/kg/d	2.69 x10 ⁻⁸ (41 - < 51 y)	
	mg/kg/d	2.63 x10 ⁻⁸ (51 - < 61 y)	
	mg/kg/d	2.75 x10 ⁻⁸ (≥ 61 y)	
Background potato	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background root vegetables	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background bulbous vegetables (onion, etc.)	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background fruiting vegetables	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background cabbage	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background leafy vegetables	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background legumes	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background beef	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background offal	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background milk	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background butter	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background eggs	mg/kg fw	2.5 x10 ⁻⁶	Poma et al. (2018)
Background outdoor air	mg/m ³	1.34x10 ⁻¹⁰	Degrendele et al. (2018)
Background indoor air	mg/m ³	6.1x10 ⁻⁹	Wemken et al (2019)
Background drinking water	mg/m ³	2x10 ⁻⁴	Brueller et al. (2018)

Plant	BCF or BCF model	Source
potatoes		
potatoes	7.15	Wang et al. (2016)
root and tuber vegetables		
carrots	0.57	Wang et al. (2011)
salsify	0.50	Read-across average carrot/radish
other root vegetables (such as radish)	0.43	Wang et al. (2011)
bulbous vegetables		
bulbous vegetables (such as onion)	7.1	Wang et al. (2011, 2016)
leek	7.1	Read-across onion
fruiting vegetables		
tomato	2.5	Navarro et al. (2017)
cucumber	2.5	Read-across tomato
other fruiting vegetables (such as peppers)	2.5	Read-across tomato
cabbages		
cabbage	1.1	Wang et al. (2011)
cauliflower and broccoli	0.57	Wang et al. (2011)
sprouts	0.86	Read-across average cabbage/cauliflower
leafy vegetables		
lettuce	0.94	Bizkarguenaga et al. (2016), Wang et al. (2011)
lamb's lettuce	0.78	Read-across average lettuce/spinach
endive	0.78	Read-across average lettuce/spinach
spinach	0.61	Navarro et al. (2017), Wu et al. (2018)
chicory	0.78	Read-across average lettuce/spinach
celery	0.78	Read-across average lettuce/spinach
legumes		
beans	1	Read-across peas
peas	1	Wang et al. (2011)
grasses		
grass	9.2	Parolini et al. (2012)
cereals		
maize	0.0038	Huang et al (2011)