

Chemical	CAS #	Surrogate Chemical	Surrogate CAS #	Rationale
Acenaphthylene	208-96-8	Acenaphthene	83-32-9	Acenaphthene is used in many studies alongside Acenaphthylene and vice versa due to their almost identical structure and function.
Barban	101-27-9	Linuron	330-55-2	Structurally similar with comparable modes of herbicidal action.
Benzo(g,h,i)perylene	191-24-2	Pyrene	129-00-0	Though Benzo(a)pyrene (BaP) is more structurally similar than pyrene, the research given for BghiP determines that it is not as harmful as BaP. Pyrene remains a conservative surrogate. "Experimental results demonstrate lower human genotoxicity profile of B[ghi]P than for benzo[a]pyrene. ANIMAL STUDIES: Benzo(ghi)perylene showed no tumorigenic effect in the respiratory tracts of rats when given at doses of 5 mg."
Bromodiphenyl Ether (p-BDE)	101-55-3	BDE-47	5436-43-1	Closest similar substance with a corresponding EPA IRIS RfC toxicity factor.
Carbazole	86-74-8	Fluorene	86-73-7	Per recommendation by EPA Region 4 from the EPA-ORD Health Risk Tech Support Center Correspondence dated March 8, 2023. Fluorene has an IRIS RfD.
Chloroaniline	27134-26-5	Chloroaniline, p-	106-47-8	Similar in all regards. Has a corresponding EPA PPRTV RfD toxicity factor.
Chloroaniline, 2-	95-51-2			
Chloroaniline, 3-	108-42-9			
Chlorohexane	544-10-5	Hexane, n-	110-54-3	n-Hexane is the closest chemical in relation to Chlorohexane with toxicity factors available and is still a conservative surrogate.
Chlorophenol, 3-	108-43-0	Chlorophenol, 2-	95-57-8	Similar in all regards. Has a corresponding IRIS RfD toxicity factor.
Chlorophenol, 4-	106-48-9			
Chlorophenyl phenyl ether, 4-	7005-72-3	Chlorobenzilate	510-15-6	Though Chlorobenzilate is not the first choice when it comes to surrogates, it's the closest surrogate to 4-CDE with approved toxicity factors available. It is also an EPA recommended surrogate for similar chemicals like 4,4'-DCBP.
Dichlorobenzene, 1,3-	541-73-1	Dichlorobenzene, 1,4-	106-46-7	EPA Region 4 recommends that 1,3-DCB be evaluated using the non-cancer toxicity values of its surrogate 1,4-DCB only and that cancer risk not be calculated using the cancer-based surrogate toxicity values.
Dichlorophenol, 2,3-	576-24-9	Dichlorophenol, 2,4-	120-83-2	Similar in all regards. Has a corresponding EPA IRIS RfD toxicity factor.
Dichlorophenol, 2,5-	583-78-8			
Dichlorophenol, 2,6-	87-65-0			
Dichloropropane, 2,2-	594-20-7	Dichloropropane, 1,2-	78-87-5	Similar in all regards. Has corresponding PPRTV RfD and IRIS RfC toxicity factors.
Dichloropropene, 1,1-	563-58-6	Dichloropropene, 1,3-	542-75-6	Dichloropropene, 1,3- is the only dichloropropene with toxicity values. These values are provided by the EPA IRIS database.
Dichloropropene, 1,2-	6923-20-3			
Dichloropropene, 2,3-	78-88-6			
Dichloropropene, cis-1,3-	10061-01-5	Dichloropropene, 1,3-	542-75-6	The stereoisomers of 1,3-Dichloropropene should be summed and compared to 1,3-Dichloropropene's calculated values for screening purposes, as the IRIS toxicity factors for 1,3-Dichloropropene are based on an almost 50:50 mixture of the two stereoisomers.
Dichloropropene, trans-1,3-	10061-02-6			
Dichlorprop	120-36-5	2,4-D	94-75-7	Both Dichlorprop and 2,4-D are chlorophenoxy herbicides. They are structurally and toxicologically similar as they have close to the same function. 2,4-D has an IRIS RfD toxicity factor.
Dimethyl phthalate	131-11-3	Diethyl phthalate	84-66-2	Similar in all regards. Has a corresponding IRIS RfD toxicity factor.
Dinitro-o-cresol, 4,6-*	534-52-1	Dinoseb	88-85-7	Dinoseb and Dinitro-o-cresol, 4,6- have a historical relationship. Dinoseb was developed as a closely related variant of DNOC. They use the same mode of action and are extremely similar structurally.
Endosulfan I	959-98-8	Endosulfan	115-29-7	The isomers, alpha- and beta-Endosulfan, should be summed and compared to Endosulfan's calculated values.
Endosulfan II	33213-65-9			
Endrin aldehyde	7421-93-4	Endrin	72-20-8	Endrin Ketone and Aldehyde are metabolites of Endrin. Endrin has a corresponding IRIS RfD.
Endrin ketone	53494-70-5			
Ethyltoluene, 4-	622-96-8	Ethylbenzene	100-41-4	Similar alkylbenzenes. Ethylbenzene contains a corresponding IRIS RfC and PPRTV RfD.
Isodrin	465-73-6	Aldrin	309-00-2	Structurally extremely similar, as it is an isomer. Aldrin has an IRIS RfD toxicity factor.
Methylcyclohexane *	108-87-2	Cyclohexane	110-82-7	Closest similar substance with a corresponding IRIS RfC toxicity factor.
3-Nitroaniline	99-09-2	4-Nitroaniline	100-01-6	Similar in all regards. Has corresponding PPRTV RfD and PPRTV RfC toxicity factors.
2-Nitroaniline*	88-74-4			
Nitrophenol, 2-	88-75-5			
Nitrophenol, 3-	554-84-7	Dinitrophenol, 2,4-	51-28-5	2,4-Dinitrophenol is similar in structure to 2-Nitrophenol, 3-Nitrophenol, and 4-Nitrophenol. It is also the closest in structure with noncancer toxicity factors. Though Nitrobenzene has toxicity factors, it doesn't have a phenol group like the others.
Nitrophenol, 4-	100-02-7			
Phenanthrene	85-01-8	Pyrene	129-00-0	Pyrene is a similar PAH with the lowest reference dose, making it a conservative surrogate.
Tetrachlorophenol, 2,3,4,5-	4901-51-3	Tetrachlorophenol, 2,3,4,6-	58-90-2	Tetrachlorophenol, 2,3,4,6- is the only Tetrachlorophenol with a toxicity factor. It has a listed, corresponding IRIS RfD.
Tetrachlorophenols	25167-83-3			
Thionazin	297-97-2	Quinalphos	13593-03-8	Structurally similar organophosphate insecticides with phosphorothioate functional groups. Quinalphos has a corresponding IRIS RfD.
Trichlorobenzene, 1,2,3-	87-61-6	Trichlorobenzene, 1,2,4-	120-82-1	Similar in all regards. Has corresponding IRIS RfD and PPRTV RfC toxicity factors.
Chlordane, cis-	5103-71-9	Chlordane, Technical	12789-03-6	These are the primary compounds or primary metabolites of Technical Chlordane.
Chlordane, trans-	5103-74-2			
Nonachlor, trans-	39765-80-5			
Oxychlordane	27304-13-8	Hexachlorocyclohexane, Technical	608-73-1	These are stereoisomers found in Technical Hexachlorocyclohexane.
Hexachlorocyclohexane, Delta- *	319-86-8			
Hexachlorocyclohexane, Epsilon	6108-10-7			

Note: Only noncancer toxicity factors should be used when utilizing chemical surrogates. Determining chemical carcinogenesis requires more complex considerations.

Surrogate toxicity factors introduce additional uncertainty. This uncertainty should be addressed in the risk characterization portion of a risk assessment.

* : This substance has a U.S. EPA provisional peer-reviewed screening toxicity factor only. Deriving cleanup levels using screening toxicity factors is acceptable by the EPD with a discussion of its uncertainty; however, an optional surrogate with a higher-tiered non-cancer toxicity factor is provided for use in the calculation of risk-based cleanup levels. An alternative surrogate may be proposed using EPA's CompTox Chemical Dashboard.