Appendix G

Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information

Appendix G. Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information

Appendix G provides detail and supporting information on the oral reference values (RfVs) and oral slope factors (OSFs) that were identified in Chapter 9 of this assessment.[1] Section G.1 provides detail on the criteria used to select sources of RfVs and OSFs for chemicals used or detected in hydraulic fracturing processes, and lists all sources of RfVs and OSFs that were considered for this study. Section G.2 provides a glossary of the toxicity value terminology that is used by these various sources. Lastly, all of the RfVs and OSFs collected from these sources are provided in Table G-1 and Table G-2. Tables G-1a through G-1d show the available RfVs and OSFs for chemicals used in hydraulic fracturing fluids, and Tables G-2a through G-2d show the available RfVs and OSFs for chemicals detected in hydraulic fracturing flowback and wastewater. These tables provide cancer weight-of-evidence (WOE) characterizations for these chemicals where available, and indicate whether each chemical has available data on physicochemical properties or occurrence.

G.1. Criteria for Selection and Inclusion of Reference Value (RfV) and Oral Slope Factor (OSF) Data Sources

The criteria listed below were used to evaluate the quality of RfVs and OSFs considered for use in the hazard analyses conducted in Chapter 9. These criteria were originally outlined in the hydraulic fracturing research plan (U.S. EPA, 2011a) and interim progress report (U.S. EPA, 2012c). Only data sources that met these criteria were considered of sufficient quality to be included in the analyses.

The following criteria had to be met for a source to be deemed of sufficient quality:

1) The body or organization generating or producing the peer-reviewed RfVs, peer-reviewed OSFs, or peer reviewed qualitative assessment must be a governmental or intergovernmental body.
    a. Governmental bodies include sovereign states, and federated states/units.
    b. Intergovernmental bodies are those whose members are sovereign states, and the subdivisions or agencies of such intergovernmental bodies. The United Nations is an example of an intergovernmental body. The International Agency for Research on Cancer (IARC) is an agency of the World Health Organization (WHO), which is itself an agency of the United Nations. Thus, IARC is considered a subdivision of the United Nations.

[1] As defined in Chapter 9, the term RfV refers to reference values for noncancer effects occurring via the oral route of exposure and for chronic durations, except where noted.

2) The data source must include peer-reviewed RfVs, peer-reviewed OSFs, or peer reviewed qualitative assessments.
    a. A committee that is established to derive the RfVs, OSFs, or qualitative assessments can have members of that same committee provide the peer review, so long as either the entire committee, or members of the committee who did not participate in the derivation of a specific section of a work product, conduct the review.
    b. Peer reviewers who work for grantees of the organization deriving the RfVs, OSFs, or qualitative assessments are generally allowed, and this will not be considered to constitute a conflict/duality of interest.
    c. Peer reviewers may work in the same or different office, so long as they did not participate in any way in the development of the product, and these individuals must be free of conflicts/duality of interest with respect to the chemical(s) assigned.
        i. For instance, peer reviewers for Program X, conducted by Office A, may also be employed by Office A so long as they did not participate in the creation of the Program X product they are reviewing.

3) The RfVs, OSFs, or qualitative assessments must be based on peer-reviewed scientific data.
    a. There are cases where industry reports that were not published in a peer-reviewed, scholarly journal may be used, if the industry report has been adequately peer-reviewed by an external body (external to the group generating the report, and external to the group generating the peer-reviewed RfVs, peer-reviewed OSFs, or peer-reviewed qualitative assessment) that is free of conflicts/dualities of interest.

4) The RfVs, OSFs, or qualitative assessments must be focused on protection of the general public.
    a. Sources that are focused on workers are not appropriate as workers are assumed to accommodate additional risk than the general public due to their status as workers.

5) The body generating the values or qualitative assessments must be free of conflicts of interest with respect to the chemicals for which it derives RfVs, OSFs, or qualitative assessments.
    a. If a body generating the RfVs, OSFs, or qualitative assessments accepts funding from an interested party (i.e., a company or organization that may be impacted by past, present, or future values or qualitative assessments), then the body has a conflict of interest.
    b. For instance, if a non-profit organization is funded by an industry trade group, and the non-profit generates RfVs, OSFs, or qualitative assessments for chemicals that trade group is interested in, then the non-profit is considered to have a conflict of interest with respect to those chemicals.

It is important to note that having a conflict/duality of interest for one chemical is sufficient to disqualify the entire database, as it is assumed that conflicts/dualities of interest may exist for other chemicals as well.

G.1.1. Included Sources

We applied our criteria to 16 different sources of RfVs and/or OSFs. After application of our criteria, we were left with eight sources. For those sources which did not meet our criteria, we provide an explanation of why they were excluded.

The following sources were evaluated, met our criteria, and were selected as sources of reference doses or cancer slope factors for this analysis:

- **U.S. EPA Integrated Risk Information System (IRIS)**
- **U.S. EPA Human Health Benchmarks for Pesticides (HHBP)**
- **U.S. EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs)**
- **U.S. Agency for Toxic Substances and Disease Registry (ATSDR) Minimum Risk Levels (MRLs)**
- **California EPA Toxicity Criteria Database**
- **International Programme On Chemical Safety (IPCS) Concise International Chemical Assessment Documents (CICAD)**

The following sources were evaluated, met our criteria, and were selected as sources of qualitative cancer classifications:

- **International Agency for Research on Cancer (IARC)**
- **US National Toxicology Program Report on Carcinogens (RoC)**

RfVs and/or OSFs from these data sources are listed in Tables G-1a through G-1d for chemicals used in hydraulic fracturing fluid formulation, and Tables G-2a through G-2d for chemicals reported in hydraulic fracturing flowback and produced water.

In addition, Table G-1 and Table G-2 also list the EPA's drinking water maximum contaminant levels (MCLs) and maximum contaminant goal levels (MCLG) when available. These values are generally based on IRIS values, and are treatment-based. MCL and MCLG values are listed for reference only, and were not considered in the hazard analysis presented in Chapter 9.

G.1.2. Excluded Sources

- **American Conference of Governmental Industrial Hygienists:** The assessments derived by this body are specific to workers and are not generalizable to the general public. In addition, this body is not a governmental or intergovernmental body. Thus, these values were excluded based on criteria 1 and 4.
- **European Chemicals Bureau, Classification and Labeling Annex I of Directive 67/548/EEC:** These assessments are not based on peer-reviewed values, but are based on data supplied by manufacturers. Further, the enabling legislation states that "Manufacturers, importers, and downstream users shall examine the information…to ascertain whether it is adequate, reliable and scientifically valid for the purpose of the

evaluation…" This clearly demonstrates that the data and the evaluation are not required to be peer-reviewed. Thus, these values were excluded based on criterion 2.

- **Toxicology Excellence for Risk Assessment's (TERA's) International Toxicity Estimates for Risk Assessment (ITER):** The ITER database is developed by TERA a 501(c)(3) non-profit. TERA accepts funding from various sources, including interested parties that may be impacted by their assessment work. Thus, ITER is excluded based on criteria 1 and 5.
- **Other U.S. states:** The EPA evaluated values from all states that had values reported on their websites. If a state's values were determined to be largely duplicative of the EPA's values (e.g., the state adopts EPA values, such as the regional screening levels, and does not typically generate its own peer-reviewed values), that state's values were no longer considered. The EPA contacted those states whose values were determined to not be duplicative of EPA's values, and confirmed whether or not a peer review process was used to develop the state's values. The EPA determined that of the states with values not duplicative of the EPA's values, only California's values met all of the EPA's criteria for this report. Other states with publicly accessible RfVs and/or OSFs include: Alabama, Florida, Hawaii, and Texas.
- **WHO Guidelines for Drinking-Water Quality:** The WHO Guidelines' values are not RfVs, but rather drinking water values.

G.2. Glossary of Toxicity Value Terminology

This section defines the toxicity values and qualitative cancer classifications that are frequently found in the sources identified above.

Lowest-observed-adverse-effect level (LOAEL): The lowest exposure level at which there are biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group. Source: U.S. EPA (2011c).

Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level. Source: OEHHA (2012).

Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards. Source: U.S. EPA (2014b).

Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals. Source: U.S. EPA (2014b).

Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse),

noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects.

- **Chronic MRL:** Duration of exposure is 365 days or longer.
- **Intermediate MRL:** Duration of exposure is >14 to 364 days.
- **Acute MRL**: Duration of exposure is 1 to 14 days.

Source: ATSDR (2009).

No-observed-adverse-effect level (NOAEL): The highest exposure level at which there are no biologically significant increases in the frequency or severity of adverse effect between the exposed population and its appropriate control; some effects may be produced at this level, but they are not considered adverse or precursors of adverse effects. Source: U.S. EPA (2011c).

Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100. Source: U.S. EPA (2011c).

Reference dose (RfD) (U.S. EPA IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a NOAEL, LOAEL, or benchmark dose, with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments.

- **Chronic RfD:** Duration of exposure is up to a lifetime.
- **Subchronic RfD (sRFD)**: Duration of exposure is up to 10% of an average lifespan.

Source: U.S. EPA (2011c).

Reference dose (RfD) (U.S. EPA HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for IRIS and PPRTV RfD determination. Source: U.S. EPA (2015e).

Tolerable daily intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk. Source: WHO (2015).

Weight-of-evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans.

- **EPA 1986 guidelines:** Under the EPA's 1986 risk assessment guidelines, the WOE was described by categories "A through E," with Group A for known human carcinogens through Group E for agents with evidence of noncarcinogenicity. Five standard WOE descriptors were used:
    - A: Human carcinogen
    - B1: Probable human carcinogen—based on limited evidence of carcinogenicity in humans and sufficient evidence of carcinogenicity in animals
    - B2: Probable human carcinogen—based on sufficient evidence of carcinogenicity in animals
    - C: Possible human carcinogen
    - D: Not classifiable as to human carcinogenicity
    - E: Evidence of noncarcinogenicity for humans

  Source: U.S. EPA (2011c).

- **EPA 1996 proposed guidelines:** The EPA's 1996 proposed guidelines outlined a major change in the way hazard evidence was weighted in reaching conclusions about the human carcinogenic potential of agents. These guidelines replaced the WOE letter categories with the use of standard descriptors of conclusions incorporated into a brief narrative. Three categories of descriptors with the narrative were used:
    - Known/likely
    - Cannot be determined
    - Not likely

  Source: U.S. EPA (1996).

- **EPA 1999 guidelines:** The 1999 guidelines adopted a framework incorporating hazard identification, dose-response assessment, exposure assessment, and risk characterization with an emphasis on characterization of evidence and conclusions in each part of the assessment. Five descriptors summarizing the WOE in the narrative were used:
    - Carcinogenic to humans
    - Likely to be carcinogenic to humans
    - Suggestive evidence of carcinogenicity, but not sufficient to assess human carcinogenic potential
    - Data are inadequate for an assessment of human carcinogenic potential
    - Not likely to be carcinogenic to humans

  Source: U.S. EPA (1999).

- **EPA 2005 guidelines:** The approach outlined in the EPA's 2005 guidelines for carcinogen risk assessment considers all scientific information in determining whether and under what conditions an agent may cause cancer in humans and provides a narrative approach to

characterize carcinogenicity rather than categories. Five standard WOE descriptors are used as part of the narrative:

- Carcinogenic to humans
- Likely to be carcinogenic to humans
- Suggestive evidence of carcinogenic potential
- Inadequate information to assess carcinogenic potential
- Not likely to be carcinogenic to humans

Source: U.S. EPA (2011c).

- **IARC Monographs on the evaluation of carcinogenic risks to humans**: The IARC classifies carcinogen risk as a matter of scientific judgement that reflects the strength of the evidence derived from studies in humans, in experimental animals, from mechanistic data, and from other relevant data. Five WOE classifications are used:
  - Group 1: Carcinogenic to humans
  - Group 2A: Probably carcinogenic to humans
  - Group 2B: Possibly carcinogenic to humans
  - Group 3: Not classifiable as to its carcinogenicity to humans
  - Group 4: Probably not carcinogenic to humans

  Source: IARC (2015).
- **NTP:** The NTP describes the results of individual experiments on a chemical agent and notes the strength of the evidence for conclusions regarding each study. Negative results, in which the study animals do not have a greater incidence of neoplasia than control animals, do not necessarily mean that a chemical is not a carcinogen, inasmuch as the experiments are conducted under a limited set of conditions. Positive results demonstrate that a chemical is carcinogenic for laboratory animals under the conditions of the study and indicate that exposure to the chemical has the potential for hazard to humans. For each separate experiment, one of the following five categories is selected to describe the findings. These categories refer to the strength of the experimental evidence and not to potency or mechanism.
  - Clear evidence of carcinogenic activity
  - Some evidence of carcinogenic activity
  - Equivocal evidence of carcinogenic activity
  - No evidence of carcinogenic activity
  - Inadequate study of carcinogenic activity

  Source: NTP (2014a).
- **The RoC** is a congressionally mandated, science-based, public health report that identifies agents, substances, mixtures, or exposures (collectively called "substances") in our

environment that may potentially put people in the United States at increased risk for cancer. NTP prepares the RoC on behalf of the Secretary of the Health and Human Services. The listing criteria in the RoC Document are:

- Known to be a human carcinogen
- Reasonably anticipated to be a human carcinogen

Source: NTP (2014b).

G.3. Tables

Table G-1a. Chemicals reported to be used in hydraulic fracturing fluids, with available federal chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by IRIS reference dose (RfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

				IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
Chemical Name	**CASRN**	**Frac-Focus data available**	**Physico-chemical data available**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic oral MRL[d] (mg/kg-day)**	**Chronic RfD[e] (mg/kg-day)**	**Public health goal[f] (MCLG) (mg/L)**	**MCL[g] (mg/L)**
Acrylamide	79-06-1	x	x	0.002	0.5	"Likely to be carcinogenic to humans"	--	--	--	0.001	--	0	--
Propargyl alcohol	107-19-7	x	x	0.002	--	--	--	--	--	--	--	--	--
Furfural	98-01-1	x	x	0.003	--	--	--	--	--	--	0.01	--	--
Benzene	*71-43-2*	*x*	*x*	*0.004*	*0.015-0.055*	*A*	--	--	--	*0.0005*	--	*0*	*0.005*
Dichloromethane	*75-09-2*	*x*	*x*	*0.006*	*0.002*	*"Likely to be carcinogenic in humans"*	--	--	--	*0.06*	--	*0*	*0.005*
Naphthalene	*91-20-3*	*x*	*x*	*0.02*	--	"Data are inadequate to assess human carcinogenic potential"	--	--	--	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
1,4-Dioxane	*123-91-1*	*x*	*x*	*0.03*	*0.1*	*"Likely to be carcinogenic to humans"*	--	--	--	*0.1*	--	--	--
Sodium chlorite	7758-19-2	x		0.03	--	*"Data are inadequate to assess human carcinogen-icity"*	--	--	--	--	--	1	0.8
Chlorine dioxide	10049-04-4	x		0.03	--	"Data are inadequate to assess human carcinogen-icity"	--	--	--	--	--	--	--
1,3-Dichloropropene	542-75-6	x	x	0.03	0.05	"Likely to be a human carcinogen"	--	--	--	0.03	--	--	--
Bisphenol A	80-05-7	x	x	0.05	--	--	--	--	--	--	--	--	--
Toluene	*108-88-3*	*x*	*x*	*0.08*	--	*"Inadequate information to assess the carcinogenic potential"*	--	--	--	--	--	*1*	*1*
Ethylbenzene	*100-41-4*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	*0.7*	*0.7*

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
1-Butanol	71-36-3	x	x	0.1	--	D	--	--	--	--	--	--	--
Cumene	*98-82-8*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
Acetophenone	*98-86-2*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
2-Butoxyethanol	111-76-2	x	x	0.1	--	"Not likely to be carcino-genic to humans"	--	--	--	--	--	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.2*	--	*"Data are inadequate to assess the carcinogenic potential"*	--	--	--	*0.2*	--	*10*	*10*
Formaldehyde	50-00-0	x	x	0.2	--	B1	--	--	--	0.2	--	--	--
Phenol	*108-95-2*	*x*	*x*	*0.3*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
2-Methyl-1-propanol	78-83-1	x	x	0.3	--	--	--	--	--	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Acetone	*67-64-1*	*x*	*x*	*0.9*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Ethyl acetate	141-78-6	x	x	0.9	--	--	--	--	IN	--	--	--	--
Ethylene glycol	*107-21-1*	*x*	*x*	*2*	--	--	--	--	--	--	--	--	--
Methanol	*67-56-1*	*x*	*x*	*2*	--	--	--	--	--	--	--	--	--
Benzoic acid	65-85-0	x	x	4	--	D	--	--	--	--	--	--	--
Aniline	62-53-3	x	x	--	0.0057	B2	0.007	--	--	--	--	--	--
Benzyl chloride	100-44-7	x	x	--	0.17	B2	0.002	--	--	--	--	--	--
(E)-Crotonaldehyde	123-73-9	x	x	--	--	C	0.001	--	--	--	--	--	--
N,N-Dimethylformamide	68-12-2	x	x	--	--	--	0.1	--	IN	--	--	--	--
Epichlorohydrin	106-89-8	x	x	--	0.0099	B2	0.006	--	--	--	--	0	--
1,2-Propylene glycol	*57-55-6*	*x*	*x*	--	--	--	*20*	--	*NL*	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
2-(2-Butoxyethoxy) ethanol	112-34-5	x	x	--	--	--	0.03	--	IN	--	--	--	--
Hexanedioic acid	124-04-9	x	x	--	--	--	2	--	--	--	--	--	--
Quinoline	91-22-5	x	x	--	3	"Likely to be carcinogenic in humans"	--	--	--	--	--	--	--
Ethylenediamine	107-15-3	x	x	--	--	D	0.09	--	IN	--	--	--	--
Formic acid	*64-18-6*	*x*	*x*	--	--	--	*0.9*	--	*IN*	--	--	--	--
Sodium chlorate	7775-09-9	x		--	--	--	--	--	--	--	0.03	--	--
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1	x		--	--	--	--	--	--	--	0.44	--	--
Benzenesulfonic acid, C10-16-alkyl derivs.	68584-22-5	x		--	--	--	--	--	--	--	0.5	--	--
Ammonium phosphate	7722-76-1	x		--	--	--	49	--	IN	--	--	--	--
Didecyldimethylammonium chloride	7173-51-5	x	x	--	--	--	--	--	--	--	0.1	--	--
2-(Thiocyano methylthio)benzothiazole	21564-17-0	x	x	--	--	--	--	--	--	--	0.01	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Mineral oil - includes paraffin oil	8012-95-1	x		--	--	--	3	--	IN	--	--	--	--
Trisodium phosphate	7601-54-9	x		--	--	--	49	--	IN	--	--	--	--
Triphosphoric acid, pentasodium salt	7758-29-4	x		--	--	--	49	--	IN	--	--	--	--
Aluminum	*7429-90-5*	*x*		--	--	--	*1*	--	*IN*	*1*	--	--	--
Phosphoric acid	7664-38-2	x		--	--	--	48.6	--	IN	--	--	--	--
Iron	*7439-89-6*	*x*		--	--	--	*0.7*	--	*IN*	--	--	--	--
Tricalcium phosphate	7758-87-4	x		--	--	--	49	--	IN	--	--	--	--
Bis(2-chloroethyl) ether	*111-44-4*	*x*	*x*	--	*1.1*	*B2*	--	--	--	--	--	--	--
Dodecylbenzenesulfonic acid	27176-87-0	x	x	--	--	--	--	--	--	--	0.5	--	--
Hydrazine	302-01-2	x		--	3	B2	--	--	--	--	--	--	--
Tetrasodium pyrophosphate	7722-88-5	x		--	--	--	49	--	IN	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Potassium phosphate, tribasic	7778-53-2	x		--	--	--	49	--	IN	--	--	--	--
Sodium trimetaphosphate	7785-84-4	x		--	--	--	49	--	IN	--	--	--	--
Arsenic	*7440-38-2*			*0.0003*	*1.5*	*A*	--	--	--	*0.0003*	--	*0*	*0.010*
Phosphine	7803-51-2			0.0003	--	D	--	--	--	--	--	--	--
Acrolein	*107-02-8*		*x*	*0.0005*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Chromium (VI)	*18540-29-9*			*0.003*	--	*A (inhaled); D(oral)*	--	--	--	*0.0009*	--	--	--
Di(2-ethylhexyl) phthalate	*117-81-7*		*x*	*0.02*	*0.014*	*B2*	--	--	--	*0.06*	--	*0*	*0.006*
Chlorine	*7782-50-5*			*0.1*	--	--	--	--	--	--	--	--	--
Styrene	100-42-5		x	0.2	--	--	--	--	--	--	--	0.1	0.1

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Zinc	*7440-66-6*			*0.3*	--	*"Inadequate information to assess carcinogenic potential"*	--	--	--	*0.3*	--	--	--
Acrylic acid	79-10-7		x	0.5	--	--	--	--	IN	--	--	--	--
Chromium (III)	*16065-83-1*			*1.5*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Phthalic anhydride	85-44-9		x	2	--	--	--	--	--	--	--	--	--
Cyclohexanone	108-94-1		x	5	--	--	--	--	IN	--	--	--	--
1,2-Propylene oxide	75-56-9		x	--	0.24	B2	--	--	--	--	0.001	--	--
2-(2-Ethoxyethoxy) ethanol	111-90-0		x	--	--	--	0.06	--	IN	--	--	--	--
Tributyl phosphate	126-73-8		x	--	--	--	0.01	0.009	LI	0.08	--	--	--
2-Methoxyethanol	109-86-4		x	--	--	--	0.005	--	IN	--	--	--	--
Polyphosphoric acids, sodium salts	68915-31-1			--	--	--	49	--	IN	--	--	--	--
Phosphoric acid, diammonium salt	7783-28-0			--	--	--	49	--	IN	--	--	--	--

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Sodium pyrophosphate	7758-16-9			--	--	--	49	--	IN	--	--	--	--
Phosphoric acid, aluminium sodium salt	7785-88-8			--	--	--	49	--	IN	--	--	--	--

ATSDR = Agency for Toxic Substances and Disease Registry; CASRN = Chemical Abstract Service Registry Number; IRIS = Integrated Risk Information System; PPRTV = Provisional Peer Reviewed Toxicity Values; HHBP = Human Health Benchmarks for Pesticides

[a] Reference dose (RfD) (IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Chronic RfD: Duration of exposure is up to a lifetime.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

[c] Weight of evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. See glossary for details.

[d] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Chronic MRL: Duration of exposure is 365 days or longer.

[e] Reference dose (RfD) (HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for RfD determination.

[f] Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals.

[g] Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

Table G-1b. Chemicals reported to be used in hydraulic fracturing fluids, with available state chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by California EPA maximum allowable daily level (MADL). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
Ethylene oxide	75-21-8	x	x	20	0.31
Benzene	*71-43-2*	*x*	*x*	*24*	*0.1*
N-Methyl-2-pyrrolidone	872-50-4	x	x	17000	--
Acrylamide	79-06-1	x	x	140	4.5
Aniline	62-53-3	x	x	--	0.0057
Benzyl chloride	100-44-7	x	x	--	0.17
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*0.027*
Epichlorohydrin	106-89-8	x	x	--	0.08
Ethylbenzene	*100-41-4*	*x*	*x*	--	*0.011*
Nitrilotriacetic acid	139-13-9	x	x	--	0.0053
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	x	x	--	0.01
Thiourea	62-56-6	x	x	--	0.072
Bis(2-chloroethyl) ether	*111-44-4*	*x*	*x*	--	*2.5*
1,3-Butadiene	106-99-0	x	x	--	0.6
Hydrazine	302-01-2	x		--	3
1,3-Dichloropropene	542-75-6	x	x	--	0.091
Dichloromethane	*75-09-2*	*x*	*x*	--	*0.014*
Lead	*7439-92-1*			*0.5*	*0.0085*
Chromium (VI)	*18540-29-9*			*8.2*	*0.5*
2-Methoxyethanol	109-86-4		x	63	--
2-Ethoxyethanol	110-80-5		x	750	--

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
Di(2-ethylhexyl) phthalate	*117-81-7*		*x*	*20 (neonate male) 58 (infant male) 410 (adult)*	*0.003*
1,2-Propylene oxide	75-56-9		x	--	0.24
Arsenic	*7440-38-2*			--	*9.5*

[a] Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100.

Table G-1c. Chemicals reported to be used in hydraulic fracturing fluids, with available international chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by CICAD reference dose (TDI, or tolerable daily intake). An "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physicochemical data available	IPCS Chronic TDI[a] (mg/kg-day)
D-Limonene	5989-27-5	x	x	0.1
Potassium iodide	7681-11-0	x		0.01
Sodium iodide	7681-82-5	x		0.01
Copper(I) iodide	7681-65-4	x		0.01
Glyoxal	107-22-2	x	x	0.2
Ethylene glycol	*107-21-1*	*x*	*x*	*0.05*
N-Methyl-2-pyrrolidone	872-50-4	x	x	0.6
Strontium chloride	10476-85-4			0.13
Chromium (VI)	*18540-29-9*			*0.0009*

IPCS = International Programme on Chemical Safety; CICAD = Concise International Chemical Assessment Documents

[a] Tolerable daily intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk.

Table G-1d. Chemicals reported to be used in hydraulic fracturing fluids, with available less-than-chronic RfVs and OSFs.

Chemicals from the FracFocus database are listed first, ranked by PPRTV subchronic reference dose (sRfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus (U.S. EPA, 2015a) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Benzyl chloride	100-44-7	x	x	0.002	--	--
Epichlorohydrin	106-89-8	x	x	0.006	--	--
(E)-Crotonaldehyde	123-73-9	x	x	0.01	--	--
Benzene	*71-43-2*	*x*	*x*	*0.01*	--	--
Ethylbenzene	*100-41-4*	*x*	*x*	*0.05*	--	*0.4*
Ethylenediamine	107-15-3	x	x	0.2	--	--
N,N-Dimethylformamide	68-12-2	x	x	0.3	--	--
2-(2-Butoxyethoxy)ethanol	112-34-5	x	x	0.3	--	--
Hexane	110-54-3	x	x	0.3	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.4*	*1*	*0.4*
Antimony trioxide	1309-64-4	x		0.5	--	--
Iron	*7439-89-6*	*x*		*0.7*	--	--
Toluene	*108-88-3*	*x*	*x*	*0.8*	*0.8*	*0.02*
Formic acid	*64-18-6*	*x*	*x*	*0.9*	--	--
Hexanedioic acid	124-04-9	x	x	2	--	--
Benzoic acid	65-85-0	x	x	4	--	--
1,2-Propylene glycol	*57-55-6*	*x*	*x*	*20*	--	--
Mineral oil - includes paraffin oil	8012-95-1	x		30	--	--
Phosphoric acid	7664-38-2	x		48.6	--	--
Ammonium phosphate	7722-76-1	x		49	--	--
Trisodium phosphate	7601-54-9	x		49	--	--
Triphosphoric acid, pentasodium salt	7758-29-4	x		49	--	--

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Tricalcium phosphate	7758-87-4	x		49	--	--
Tetrasodium pyrophosphate	7722-88-5	x		49	--	--
Potassium phosphate, tribasic	7778-53-2	x		49	--	--
Sodium trimetaphosphate	7785-84-4	x		49	--	--
Acrylamide	79-06-1	x	x	--	0.01	0.001
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*5*	*0.5*
Ethylene glycol	*107-21-1*	*x*	*x*	--	*0.8*	*0.8*
Naphthalene	*91-20-3*	*x*	*x*	--	*0.6*	*0.6*
Phenol	*108-95-2*	*x*	*x*	--	*1*	--
Sodium chlorite	7758-19-2	x		--	--	0.1
Acetone	*67-64-1*	*x*	*x*	--	--	*2*
2-Butoxyethanol	111-76-2	x	x	--	0.4	0.07
Aluminum	*7429-90-5*	*x*		--	--	*1*
Formaldehyde	50-00-0	x	x	--	--	0.3
1,3-Dichloropropene	542-75-6	x	x	--	--	0.04
Dichloromethane	*75-09-2*	*x*	*x*	--	*0.2*	--
Antimony trichloride	10025-91-9			0.0004	--	--
2-Methoxyethanol	109-86-4		x	0.02	--	--
Tributyl phosphate	126-73-8		x	0.03	1.1	0.08
Acrylic acid	79-10-7		x	0.2	--	--
2-(2-Ethoxyethoxy) ethanol	111-90-0		x	0.6	--	--
Cyclohexanone	108-94-1		x	2	--	--
Polyphosphoric acids, sodium salts	68915-31-1			49	--	--
Phosphoric acid, diammonium salt	7783-28-0			49	--	--
Sodium pyrophosphate	7758-16-9			49	--	--

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Phosphoric acid, aluminium sodium salt	7785-88-8			49	--	--
Acrolein	*107-02-8*		*x*	--	--	*0.004*
Di(2-ethylhexyl) phthalate	*117-81-7*		*x*	--	--	*0.1*
Styrene	100-42-5		x	--	0.1	--
Arsenic	*7440-38-2*			--	*0.005*	--
Chromium (VI)	*18540-29-9*			--	--	*0.005*
Copper	*7440-50-8*			--	*0.01*	*0.01*
Zinc	*7440-66-6*			--	--	*0.3*

[a] Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Subchronic RfD (sRFD): Duration of exposure is up to 10% of an average lifespan.

[b] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Acute MRL: Duration of exposure is 1 to 14 days.

[c] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Intermediate MRL: Duration of exposure is >14 to 364 days.

Table G-2a. Chemicals reported to be detected in flowback or produced water, with available federal chronic RfVs and OSFs.

Chemicals are ranked by IRIS reference dose (RfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

				IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
Chemical Name	**CASRN**	**Concen-tration data available**	**Physico-chemical data available**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic RfD[a] (mg/kg-day)**	**OSF[b] (per mg/kg-day)**	**Cancer WOE character-ization[c]**	**Chronic oral MRL[d] (mg/kg-day)**	**Chronic RfD[e] (mg/kg-day)**	**Public health goal[f] (MCLG) (mg/L)**	**MCL[g] (mg/L)**
Heptachlor epoxide	1024-57-3		x	0.000013	9.1	B2	--	--	--	--	--	0	0.0002
Phosphorus	7723-14-0	x		0.00002	--	D	--	--	--	--	--	--	--
Aldrin	309-00-2		x	0.00003	17	B2	--	--	--	0.00003	--	--	--
Dieldrin	60-57-1		x	0.00005	16	B2	--	--	--	0.00005	--	--	--
Arsenic	*7440-38-2*	x		*0.0003*	*1.5*	*A*	--	--	--	*0.0003*	--	*0*	*0.010*
Lindane	58-89-9		x	0.0003	--	--	--	--	--	--	--	0.0002	0.0002
Antimony	7440-36-0	x		0.0004	--	--	--	--	IN	--	--	0.006	0.006
Acrolein	*107-02-8*		*x*	*0.0005*	--	*"Data are inadequate for an assessment of human carcinogenic potential"*	--	--	--	--	--	--	--
Cadmium	7440-43-9	x		0.0005 (water)	--	B1	--	--	--	0.0001	--	0.005	0.005
Heptachlor	76-44-8		x	0.0005	4.5	B2	--	--	--	--	--	0	0.0004

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Cyanide	57-12-5		x	0.0006	--	"Inadequate information to assess the carcinogenic potential"	--	--	--	--	--	0.2	0.2
Pyridine	110-86-1	x	x	0.001	--	--	--	--	--	--	--	--	--
Methyl bromide	74-83-9		x	0.0014	--	D	--	--	--	--	0.02	--	--
Beryllium	7440-41-7	x		0.002	--	B1	--	--	--	0.002	--	0.004	0.004
Chromium (VI)	*18540-29-9*			*0.003*	--	*A (inhaled); D(oral)*	--	--	--	*0.0009*	--	--	--
Benzene	*71-43-2*	*x*	*x*	*0.004*	*0.015-0.055*	*A*	--	--	--	*0.0005*	--	*0*	*0.005*
2-Methylnaphthalene	91-57-6	x	x	0.004	--	"Data are inadequate to assess human carcinogenic potential"	--	--	--	0.04	--	--	--
Molybdenum	7439-98-7	x		0.005	--	--	--	--	--	--	--	--	--
Silver	7440-22-4	x		0.005	--	D	--	--	--	--	--	--	--
Selenium	7782-49-2	x		0.005	--	D	--	--	--	0.005	--	0.05	0.05
Dichloromethane	*75-09-2*		*x*	*0.006*	*0.002*	*"Likely to be carcinogenic in humans"*	--	--	--	*0.06*	--	*0*	*0.005*

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
1,2,4-Trichlorobenzene	120-82-1		x	0.01	--	D	--	0.029	LI	0.1	--	0.07	0.07
Tetrachloroethylene	127-18-4		x	0.006	0.0021	"Likely to be carcinogenic in humans"	--	--	--	0.008	--	0	0.005
Chloroform	67-66-3	x	x	0.01	--	B2	--	--	--	0.01	--	--	--
Di(2-ethylhexyl) phthalate	*117-81-7*	*x*	*x*	*0.02*	*0.014*	*B2*	--	--	--	*0.06*	--	*0*	*0.006*
Naphthalene	*91-20-3*	*x*	*x*	*0.02*	--	*"Data are inadequate to assess human carcinogenic potential"*	--	--	--	--	--	--	--
2,4-Dimethylphenol	105-67-9	x	x	0.02	--	--	--	--	IN	--	--	--	--
Chlorodibromomethane	124-48-1		x	0.02	0.084	C	--	--	--	0.09	--	--	--
Bromoform	75-25-2		x	0.02	0.0079	B2	--	--	--	0.02	--	--	--
Bromodichloromethane	75-27-4		x	0.02	0.062	B2	--	--	--	0.02	--	--	--
Diphenylamine	122-39-4	x	x	0.025	--	--	--	--	IN	--	0.1	--	--
1,4-Dioxane	*123-91-1*	*x*	*x*	*0.03*	*0.1*	*"Likely to be carcinogenic to humans"*	--	--	--	*0.1*	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Pyrene	129-00-0	x	x	0.03	--	D	--	--	--	--	--	--	--
Fluoranthene	206-44-0	x	x	0.04	--	D	--	--	IN	--	--	--	--
Fluorene	86-73-7	x	x	0.04	--	D	--	--	--	--	--	--	--
m-Cresol	108-39-4	x	x	0.05	--	C	--	--	--	--	--	--	--
o-Cresol	95-48-7	x	x	0.05	--	C	--	--	IN	--	--	--	--
Toluene	*108-88-3*	*x*	*x*	*0.08*	--	*"Inadequate information to assess the carcinogenic potential"*	--	--	--	--	--	*1*	*1*
Chlorine	*7782-50-5*			*0.1*	--	--	--	--	--	--	--	--	--
Ethylbenzene	*100-41-4*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	*0.7*	*0.7*
Cumene	*98-82-8*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
Acetophenone	*98-86-2*	*x*	*x*	*0.1*	--	*D*	--	--	--	--	--	--	--
Carbon disulfide	75-15-0	x	x	0.1	--	--	--	--	--	--	--	--	--
Dibutyl phthalate	84-74-2	x	x	0.1	--	D	--	--	--	--	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Nitrite	14797-65-0	x		0.1	--	--	--	--	--	--	--	1	1
Manganese	7439-96-5	x		0.14	--	D	--	--	--	--	--	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.2*	--	*"Data are inadequate to assess the carcinogenic potential"*	--	--	--	*0.2*	--	*10*	*10*
Barium	7440-39-3	x		0.2	--	"Not likely to be carcinogenic to humans"	--	--	--	0.2	--	2	2
Boron	7440-42-8	x		0.2	--	"Data are inadequate to assess the carcinogenic potential"	--	--	--	--	--	--	--
Zinc	*7440-66-6*	x		*0.3*	--	*"Inadequate information to assess carcinogenic potential"*	--	--	--	*0.3*	--	--	--
Phenol	*108-95-2*	*x*	*x*	*0.3*	--	*"Data are inadequate to assess human carcinogenicity"*	--	--	--	--	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Strontium	7440-24-6	x		0.6	--	--	--	--	--	--	--	--	--
Methyl ethyl ketone	78-93-3		x	0.6	--	"Data are inadequate to assess carcinogenic potential"	--	--	--	--	--	--	--
Diethyl phthalate	84-66-2		x	0.8	--	D	--	--	--	--	--	--	--
Acetone	*67-64-1*	*x*	*x*	*0.9*	--	*"Data are inadequate to assess human carcinogenicity"*	--	--	--	--	--	--	--
Chromium (III)	*16065-83-1*			*1.5*	--	*"Data are inadequate to assess human carcinogenicity"*	--	--	--	--	--	--	--
Nitrate	14797-55-8	x		1.6	--	--	--	--	--	--	--	10	10
Ethylene glycol	*107-21-1*		*x*	*2*	--	--	--	--	--	--	--	--	--
Methanol	*67-56-1*		*x*	*2*	--	--	--	--	--	--	--	--	--
1,2-Propylene glycol	*57-55-6*		*x*	--	--	--	*20*	--	*NL*	--	--	--	--
Formic acid	*64-18-6*		*x*	--	--	--	*0.9*	--	*IN*	--	--	--	--
Aluminum	*7429-90-5*	*x*		--	--	--	*1*	--	*IN*	*1*	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Iron	*7439-89-6*	x		--	--	--	*0.7*	--	*IN*	--	--	--	--
Bis(2-chloroethyl) ether	*111-44-4*		*x*	--	*1.1*	*B2*	--	--	--	--	--	--	--
Benzyl alcohol	100-51-6	x	x	--	--	--	0.1	--	IN	--	--	--	--
Butylbenzene	104-51-8		x	--	--	--	0.05	--	IN	--	--	--	--
Acrylonitrile	107-13-1		x	--	0.54	B1	--	--	--	0.04	--	--	--
Phorate	298-02-2		x	--	--	--	--	--	--	--	0.0005	--	--
beta-Hexachloro cyclohexane	319-85-7		x	--	1.8	C	--	--	--	--	--	--	--
Benzo(a)pyrene	50-32-8	x	x	--	7.3	B2	--	--	--	--	--	0	0.0002
p,p'-DDE	72-55-9		x	--	0.34	B2	--	--	--	--	--	--	--
Lithium	7439-93-2	x		--	--	--	0.002	--	IN	--	--	--	--

Chemical Name	CASRN	Concen-tration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic RfD[a] (mg/kg-day)	OSF[b] (per mg/kg-day)	Cancer WOE character-ization[c]	Chronic oral MRL[d] (mg/kg-day)	Chronic RfD[e] (mg/kg-day)	Public health goal[f] (MCLG) (mg/L)	MCL[g] (mg/L)
Cobalt	7440-48-4	x		--	--	--	0.0003	--	LI	--	--	--	--
Vanadium	7440-62-2	x		--	--	--	0.00007	--	IN	--	--	--	--
N-Nitrosodiphenylamine	86-30-6	x	x	--	0.0049	B2	--	--	--	--	--	--	--

ATSDR = Agency for Toxic Substances and Disease Registry; CASRN = Chemical Abstract Service Registry Number; IRIS = Integrated Risk Information System; PPRTV = Provisional Peer Reviewed Toxicity Values; HHBP = Human Health Benchmarks for Pesticides

[a] Reference dose (RfD) (IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Chronic RfD: Duration of exposure is up to a lifetime.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

[c] Weight of evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. See glossary for details.

[d] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Chronic MRL: Duration of exposure is 365 days or longer.

[e] Reference dose (RfD) (HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for RfD determination.

[f] Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals.

[g] Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

1

Table G-2b. Chemicals reported to be detected in flowback or produced water, with available state chronic RfVs and OSFs.

Chemicals are ranked by California EPA maximum allowable daily level (MADL). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physicochemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
Lead	*7439-92-1*	*x*		*0.5*	*0.0085*
Cadmium	7440-43-9	x		4.1	15
Chromium (VI)	*18540-29-9*			*8.2*	*0.5*
Dibutyl phthalate	84-74-2	x	x	8.7	--
Benzene	*71-43-2*	*x*	*x*	*24*	*0.1*
Acrylonitrile	107-13-1		x	--	1
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*0.027*
Ethylbenzene	*100-41-4*	*x*	*x*	--	*0.011*
Di(2-ethylhexyl) phthalate	*117-81-7*	*x*	*x*	*20 (neonate male) 58 (infant male) 410 (adult)*	*0.003*
Arsenic	*7440-38-2*	*x*		--	*9.5*
Bis(2-chloroethyl) ether	*111-44-4*		*x*	--	*2.5*
Heptachlor epoxide	1024-57-3		x	--	5.5
1,2,4-Trichlorobenzene	120-82-1		x	--	0.0036
Tetrachloroethylene	127-18-4		x	--	0.051
Indeno(1,2,3-cd)pyrene	193-39-5	x	x	--	1.2
Benzo(b)fluoranthene	205-99-2	x	x	--	1.2
Benzo(k)fluoranthene	207-08-9	x	x	--	1.2
Aldrin	309-00-2		x	--	17
beta-Hexachlorocyclohexane	319-85-7		x	--	1.5
Benzo(a)pyrene	50-32-8	x	x	--	2.9
Dibenz(a,h)anthracene	53-70-3	x	x	--	4.1
7,12-Dimethylbenz(a)anthracene	57-97-6		x	--	250
Lindane	58-89-9		x	--	1.1
Dieldrin	60-57-1		x	--	16
Chloroform	67-66-3	x	x	--	0.019

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	California	
				Oral MADL[a] (µg/day)	OSF[b] (per mg/kg-day)
p,p'-DDE	72-55-9		x	--	0.34
Bromoform	75-25-2		x	--	0.011
Bromodichloromethane	75-27-4		x	--	0.13
Heptachlor	76-44-8		x	--	4.1
N-Nitrosodiphenylamine	86-30-6	x	x	--	0.009
Safrole	94-59-7		x	--	0.22
Dichloromethane	*75-09-2*		*x*	--	*0.014*

[a] Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

[b] Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100.

Table G-2c. Chemicals reported to be detected in flowback or produced water, with available international chronic RfVs and OSFs.

Chemicals are ranked by CICAD reference dose (TDI – Tolerable Daily Intake). An "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physicochemical data available	IPCS Chronic TDI[a] (mg/kg-day)
Heptachlor	76-44-8		x	0.0001
Strontium	7440-24-6	x		0.13
Chloroform	67-66-3	x	x	0.015
Mercury	7439-97-6	x		0.002
Barium	7440-39-3	x		0.02
Beryllium	7440-41-7	x		0.002
Ethylene glycol	*107-21-1*		*x*	*0.05*
Tetrachloroethene	127-18-4		x	0.05
Chromium (VI)	*18540-29-9*			*0.0009*
Diethyl phthalate	84-66-2		x	5

IPCS = International Programme on Chemical Safety; CICAD = Concise International Chemical Assessment Documents

[a] Tolerable Daily Intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk.

Table G-2d. Chemicals reported to be detected in flowback or produced water, with available less-than-chronic RfVs and OSFs.

Chemicals are ranked by PPRTV subchronic reference dose (sRfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physicochemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Aldrin	309-00-2		x	0.00004	0.002	--
Antimony	7440-36-0	x		0.0004	--	--
Vanadium	7440-62-2	x		0.0007	--	0.01
Lithium	7439-93-2	x		0.002	--	--
Cobalt	7440-48-4	x		0.003	--	0.01
2-Methylnaphthalene	91-57-6	x	x	0.004	--	--
Methyl bromide	74-83-9		x	0.005	--	0.003
Bromodichloromethane	75-27-4		x	0.008	0.04	--
1,2,3-Trichlorobenzene	87-61-6		x	0.008	--	--
Benzene	*71-43-2*	*x*	*x*	*0.01*	--	--
p-Cresol	106-44-5	x	x	0.02	--	--
Bromoform	75-25-2		x	0.03	0.7	0.2
Ethylbenzene	*100-41-4*	*x*	*x*	*0.05*	--	*0.4*
2,4-Dimethylphenol	105-67-9	x	x	0.05	--	--
Chlorodibromomethane	124-48-1		x	0.07	0.1	--
1,2,4-Trichlorobenzene	120-82-1		x	0.09	--	0.1
Butylbenzene	104-51-8		x	0.1	--	--
Benzyl alcohol	100-51-6	x	x	0.3	--	--
Pyrene	129-00-0	x	x	0.3	--	--
Xylenes	*1330-20-7*	*x*	*x*	*0.4*	*1*	*0.4*
Iron	*7439-89-6*	*x*		*0.7*	--	--
Toluene	*108-88-3*	*x*	*x*	*0.8*	*0.8*	*0.02*
Formic acid	*64-18-6*		*x*	*0.9*	--	--
1,2-Propylene glycol	*57-55-6*		*x*	*20*	--	--

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Acrolein	*107-02-8*		*x*	--	--	*0.004*
1,4-Dioxane	*123-91-1*	*x*	*x*	--	*5*	*0.5*
Ethylene glycol	*107-21-1*		*x*	--	*0.8*	*0.8*
Di(2-ethylhexyl) phthalate	*117-81-7*	*x*	*x*	--	--	*0.1*
Naphthalene	*91-20-3*	*x*	*x*	--	*0.6*	*0.6*
Phenol	*108-95-2*	*x*	*x*	--	*1*	--
Acetone	*67-64-1*	*x*	*x*	--	--	*2*
Arsenic	*7440-38-2*	*x*		--	*0.005*	--
Chromium (VI)	*18540-29-9*			--	--	*0.005*
Copper	*7440-50-8*	*x*		--	*0.01*	*0.01*
Zinc	*7440-66-6*	*x*		--	--	*0.3*
Aluminum	*7429-90-5*	*x*		--	--	*1*
Acrylonitrile	107-13-1		x	--	0.1	0.01
Dioctyl phthalate	117-84-0	x	x	--	3	0.4
Tetrachloroethylene	127-18-4		x	--	0.008	0.008
Fluoranthene	206-44-0	x	x	0.1	--	0.4
beta-Hexachlorocyclohexane	319-85-7		x	--	0.05	0.0006
Lindane	58-89-9		x	--	0.003	0.00001
Dieldrin	60-57-1		x	--	--	0.0001
Chloroform	67-66-3	x	x	--	0.3	0.1
Strontium	7440-24-6	x		--	--	2
Tin	7440-31-5	x		--	--	0.3
Barium	7440-39-3	x		--	--	0.2
Boron	7440-42-8	x		--	0.2	0.2
Cadmium	7440-43-9	x		--	--	0.0005
Carbon disulfide	75-15-0	x	x	--	0.01	--
Heptachlor	76-44-8		x	--	0.0006	0.0001
Phosphorus	7723-14-0	x		--	--	0.0002

Chemical name	CASRN	Concen-tration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD[a] (mg/kg-day)	Acute oral MRL[b] (mg/kg-day)	Intermediate oral MRL[c] (mg/kg-day)
Diethyl phthalate	84-66-2		x	--	7	6
Dibutyl phthalate	84-74-2	x	x	--	0.5	--
Fluorene	86-73-7	x	x	--	--	0.4
Dichloromethane	*75-09-2*		*x*	--	*0.2*	--

[a] Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Subchronic RfD (sRFD): Duration of exposure is up to 10% of an average lifespan.

[b] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Acute MRL: Duration of exposure is 1 to 14 days.

[c] Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Intermediate MRL: Duration of exposure is >14 to 364 days.

G.4. References for Appendix G

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