Carbon Balance Life Cyle Impact Assessment Method

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Introduction

Critical review is an essential step in life cycle assessment (LCA) to ensure that the study methodology meets International Organization for Standardization (ISO) 14040 and ISO 14044 requirements [1, 2] and study results are reliable and credible. However, it is recognized that, in practice, there is significant variability in the detail and quality of critical review activity [3]. A survey found that while a review of methods and assumptions is often performed comprehensively, an examination of data, calculations, and quantitative results is often limited [3]. This is a significant deficiency in an era where LCA results are used as a metric for determining tax credits [4].

Mass balance checks are a recommended aspect of data validation [5]. While overall mass balances are simple to perform with a compiled life cycle inventory (LCI), calculating elemental mass balances is much more time consuming. Life cycle impact assessment (LCIA) calculations in LCA software can be leveraged to perform such elemental balances, but this capability has previously been unexplored.

This carbon balance LCIA method was created as a proof-of-concept for such a use. Using a standardized set of elementary flows, the method automatically calculates the carbon balance of the user-defined product system.

Methodology

Carbon content is calculated with the following generalized formula.

$$Carbon\ Content = \frac{\#\ Moles\ C \cdot 12.011\ g/mol\ C}{Molar\ Mass\ of\ Compound}$$

All molar mass calculations used the standard atomic mass values included in the periodic table. No adjustments are made for ions or isotopes.

The Federal LCA Commons Elementary Flows List (FEDEFL) is used as the basis for resource and emission flows in the carbon balance LCIA method [6]. This is a standardized set of elementary flows that are publicly available and widely used. Thus, using this list as the foundation of the carbon balance LCIA method means that it can be widely applicable to user-constructed openLCA models.

The list metadata does include molecular formulas; however, such metadata is not included for all flows. In the construction of this impact assessment method, these metadata gaps were filled for over 500 flows. To do this, molecular formulas were sourced from reputable chemical databases [7, 8, 9, 10, 11]. Searches were first conducted based on CAS number (if provided), then flow name, then flow synonyms (if provided). This order was designed to minimize the risk of misidentified formulas. A full accounting of the molecular formulas added to the FEDEFL metadata is provided in Appendix A: Simple Molecular Formulas.

A number of flows included in FEDEFL cannot be defined by a molecular formula. These include flows with more complex compositions, such as petroleum and canola oil, flows that represent flow categories rather than individual molecules, such as quaternary ammonium compounds and chlorofluorocarbons, and flow that are otherwise not discrete structures. The carbon content of

such flows was instead determined by the carbon contents of the individual components and their mole fractions. When specific mole fractions were not available, an average of all individual components was assumed. These components and compositions were assigned after a comprehensive literature search. The resulting carbon contents are listed in Appendix B: Complex Molecular Formulas. All calculations are documented in the accompanying FEDEFL Carbon Content Calculations file.

Use Guide

The carbon balance LCIA method is built for use in openLCA version 2. Users can access the carbon balance LCIA method by downloading the provided JSON-LD file. This file can then be imported into the user's openLCA database. To minimize possible import errors, it is recommended that users import FEDEFL into their openLCA database first. A .zolca file with the carbon balance LCIA method and FEDEFL is also provided.

Users may encounter a memory error when importing the JSON-LD file into an existing database. This can be mitigated by increasing the memory usage of openLCA through File → Preferences → Configuration.

The FEDEFL flows included are too numerous to be included in a single impact assessment category; therefore, there are five separate impact assessment categories that, together, make up the carbon balance LCIA method. An accounting of these categories and their contents are summarized in Exhibit 1.

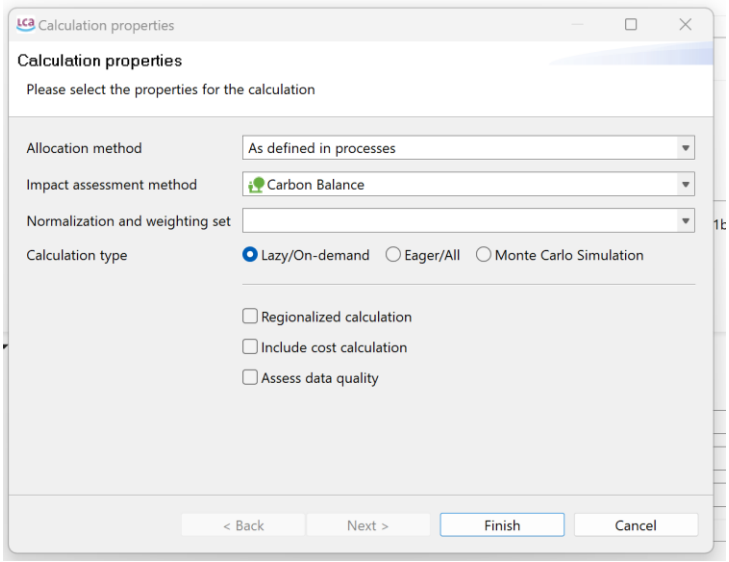
Exhibit 1. Impact Categories in Carbon Balance Impact Assessment Method

Impact Category Name	Description
Carbon Content – Resource Flows	Includes 110 FEDEFL resource flows from air, water, and ground. Characterization factors for carbon content are positive values.
Carbon Content – Emission/Air Flows	Includes 93,183 FEDEFL emission flows to air. Characterization factors for carbon content are negative values.
Carbon Content – Emission/Water Flows	Includes 107,801 FEDEFL emission flows to water. Characterization factors for carbon content are negative values.
Carbon Content – Emission/Ground Flows	Includes 94,670 FEDEFL emission flows to ground. Characterization factors for carbon content are negative values.
Carbon Content – Technosphere Flows	Empty impact category – users must add technosphere flows relevant to their modeled system. This category is included as a means to mitigate the shortcoming raised in the Limitations section. Characterization factors for carbon content may be positive or negative values based on user input.

The impact categories assign carbon content as positive or negative based on whether the flow considered is a resource or emission. The categories themselves are non-directional. The total carbon balance is complete when the impact results from each category are added together. The product system considered has carbon balance if this sum equals zero. Users must use FEDEFL elementary flows throughout their model for accurate carbon balance calculations.

Once the carbon balance LCIA method is imported, it can be used with any product system created by the user. Simply select the method when calculating results for a product system, as shown in Exhibit 2.

Exhibit 2. Display of Carbon Balance Impact Assessment Method in Product System Calculation



Assumptions

Certain assumptions were required when determining the carbon content of complex flows, including:

- No carbon content is assigned to FEDEFL flows in the biological class, which includes bacteria species and other microorganisms.
- Carbon content of biomass flows is calculated on a dry basis.
- Carbon content of natural gas is calculated based on the methane (CH_4) and carbon dioxide (CO_2) content only. Carbon content contributions from natural gas liquids (NGLs) in raw gas is excluded.
- No carbon content is assigned to land use. Carbon associated with land use change must be accounted for with other flows.
- No carbon content is assigned to soil. Carbon content of soil must be accounted for with other flows.
- Carbon content of group class flowables is assumed to be an average of flows within the group.

The carbon balance LCIA method includes 110 resource flows and nearly 300,000 emission flows. This difference in magnitude places particular importance on accurately defining the carbon content of resource flows. The carbon content of key resources flows is thus presented in Exhibit 3.

Exhibit 3. Carbon Content of Key Resource Flows

Flowable	Carbon Content (kg C/kg)	Comment(s)
Biomass	0.5	Assumed. Dry basis.
Coal	0.609	Weighted average of anthracite (1%), bituminous (55%), lignite (6%), and sub-bituminous (38%) coal by global coal reserves [12, 13].
Coal, anthracite	0.781	Average U.S. [12]
Coal, bituminous	0.70	Average U.S. [12]
Coal, lignite	0.412	Average U.S. [12]
Coal, sub-bituminous	0.503	Average U.S. [12]
Coalbed methane	0.547	Calculated assuming CH_4 content of 71.9% and CO_2 content of 3.11% at extraction, based on U.S. San Juan coalbed methane production [14]. Carbon content of any NGLs in raw gas is excluded.
Crude oil	0.846	Calculated based on IPCC net calorific value (Table 1.2) and carbon content (Table 1.3) [15].
Hardwood	0.484	Average of 22 hardwood species [16]. Dry basis.
Natural gas	0.598	Calculated assuming CH_4 content of 79.5% and CO_2 content of 0.874% at extraction, based on weighted U.S. average conventional gas production [14]. Carbon content of any NGLs in raw gas is excluded.
Oil sand	0.0884	Calculated assuming 10% bitumen in oil sands [17] and bitumen carbon content calculated based on IPCC net calorific value (Table 1.2) and carbon content (Table 1.3) [15].
Peat	0.345	Average of 14 sites (40.7%) [18] and calculated based on IPCC net calorific value (Table 1.2) and carbon content (Table 1.3) (28.2%) [15].
Primary forest	0.5	Assumed. Dry basis.
Shale gas	0.591	Calculated assuming CH_4 content of 78.8% and CO_2 content of 0.435% at extraction, based on weighted U.S. average shale gas production [14]. Carbon content of any NGLs in raw gas is excluded.
Softwood	0.51	Average of 21 softwood species [16].
Tight gas	0.567	Calculated assuming CH_4 content of 75.2% and CO_2 content of 1.45% at extraction, based on weighted U.S. average tight gas production [14]. Carbon content of any NGLs in raw gas is excluded.
Wood	0.5	Assumed. Dry basis.

The carbon contents of all complex flows are included in Appendix B: Complex Molecular Formulas.

Limitations

While this LCIA method is comprehensive in its coverage of elementary flows, there are necessarily modeling choices made in LCA that could cause the displayed carbon balance results to be misleading. This stems from the presence of technosphere flows, or product flows, in databases, which may or may not have a carbon content.

Depending on how the system boundary is drawn, not accounting for the carbon content of such technosphere flows could significantly skew the carbon balance results. An example of this is an LCA model that is not cradle-to-grave, and the functional unit or any co-products considered have a carbon content. Another example is the use of cutoff flows or input of waste products with carbon contents.

There is no standardized list of technosphere flows as there is for elementary flows. However, an empty LCIA category is included within the carbon balance LCIA method for technosphere flows. Users may add technosphere flows with carbon contents to this category, indicating carbon content with positive or negative values depending on whether the technosphere flow is a model input or output. It may be helpful to first calculate a life cycle inventory before using the carbon balance LCIA method in order to determine whether technosphere flows are inputs or outputs. If technosphere flows are used in both contexts throughout the model, the positive or negative carbon content should be assigned to the larger magnitude use. Adding technosphere flows to this empty LCIA category is not required to use the carbon balance LCIA method but may aid results interpretation.

Carbon balance results may also be inaccurate if the life cycle inventory is incomplete. Users are encouraged to use discrete chemical flows in model construction rather than group class flows for the most accurate carbon balance results. Users are also encouraged to revisit their modeling assumptions if carbon balance results seem reasonable, as it may be an indication that something deemed immaterial in the study design is important.

As with any LCIA method, some level of interpretation is required. The carbon balance of a product system may not be accurate if a co-product management strategy other than system expansion is used. This method is not meant to supplant but instead aid critical review performed by an LCA practitioner.

Future Work

This carbon balance LCIA method was developed as a proof-of-concept. Future work can thus include mass balances for other elements of interest, such as nitrogen and phosphorus. As this effort filled gaps in FEDEFL metadata for molecular formulas, construction of LCIA methods for other elemental balances should require less initial effort.

In terms of the existing carbon balance LCIA method, future work should include the addition of uncertainty to the carbon content of complex flows, or even regional characterization factors. The composition of natural gas, oil, and coal, and even the predominant biomass species vary by location. Accounting for such variations in the future would lead to a more robust LCIA method.

Future work may also include making the carbon balance LCIA method compatible with other LCA software.

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Appendix A: Simple Molecular Formulas

Exhibit A-1 documents the FEDEFL flows whose metadata did not previously include a molecular formula. Molecular formulas have been manually filled based on reputable sources in order to calculate carbon content for the carbon balance LCIA method. Unless otherwise specified, molecular formulas are sourced from reputable chemical databases [7, 8, 9, 10, 11].

Exhibit A-1. Molecular Formulas for Select Incomplete FEDEFL Entries

Flowable	CAS No.	Formula
(+)-Isobutyl D-lactate	61597-96-4	$C_7H_{14}O_3$
(1,1,3,3-Tetramethylbutyl)phenol	27193-28-8	$C_{14}H_{22}O$
(1R, 4R, 5S) 4-Hydroxy-6,6-dimethyl-3-oxabicyclo(3.1.0)hexan-2-one	73611-02-6	$C_7H_{10}O_3$
(1S,5R)-6,8-dioxabicyclo[3.2.1]octan-4-one	53716-82-8	$C_6H_8O_3$
(S)-(+)-3-Hydroxytetrahydrofuran	86087-23-2	$C_4H_8O_2$
(trans,trans)-4-(p-Tolyl)-4'-vinyl-1,1'-bi(cyclohexane)	155041-85-3	$C_{21}H_{30}$
(trans,trans)-4-Pentyl-4'-vinyl-1,1'-bi(cyclohexane)	129738-34-7	$C_{19}H_{34}$
.alpha.-D-Glucopyranoside, .beta.-D-fructofuranosyl, diacetate hexakis(2-methylpropanoate)	27216-37-1	$C_{40}H_{62}O_{19}$
[2-(2-Methoxymethylethoxy)methylethoxy]propanol	25498-49-1	$C_{10}H_{22}O_4$
1-(1,1-Dimethylethoxy)-2-methylpropane	33021-02-2	$C_8H_{18}O$
1-(2-Ethyl-butyl)-cyclohexanecarboxylic acid	381209-09-2	$C_{13}H_{24}O_2$
1(or 2)-Methoxypropanol	1320-67-8	$C_4H_{10}O_2$
1,1'-Biphenyl, nonabromo-	27753-52-2	$C_{12}HBr_9$
1,2,3,4-Tetrahydro-8-methyldibenzothiophene	54889-44-0	$C_{13}H_{14}S$
1,2,4-Benzenetricarboxylic acid, decyl octyl ester	67989-23-5	$C_{10}H_{22}O \cdot xC_9H_6O_6 \cdot xC_8H_{18}O$
1,2-Pentadiene	591-95-7	C_5H_8
1,3-Benzenediol, 4-(2-pyridinylazo)-, monosodium salt, monohydrate	16593-81-0	$C_{11}H_9N_3O_2 \cdot H_2O \cdot Na$
1,3-Dichloro-1-propene mixture with 1,2-dichloropropane	8003-19-8	$C_3H_6Cl_2 \cdot C_3H_4Cl_2$
18,19-Dinorcholestane, 5,14-dimethyl-, (5.beta.,8.alpha.,9.beta.,10.alpha.,14.beta.,20S)-	56975-84-9	$C_{27}H_{48}$
1-Aminoethanol	75-39-8	C_2H_7NO
1-Butanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	69271-91-6	$C_{12}H_{16}O_4$
1-Chloro-3-phenoxy-2-propanol	4769-73-7	$C_9H_{11}ClO_2$
1-Decene, dimer, hydrogenated	68649-11-6	$C_{20}H_{42}$
1-Hexadecene, 7,11,15-trimethyl-3-methylene-	504-96-1	$C_{20}H_{38}$
1H-Indene, 2,3-dihydrodimethyl-	53563-67-0	$C_{11}H_{14}$
1H-Indene, octahydro-	496-10-6	C_9H_{16}
1-Methylcyclohexanecarboxylic acid	1123-25-7	$CH_3C_6H_{10}CO_2H$
1-Pentene, 3,4-dimethyl-	7385-78-6	C_7H_{14}
1-Pentene, 3-methyl-	760-20-3	C_6H_{12}
1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethenyl)-, (1R,4aS,10aR)-	82276-84-4	$C_{20}H_{26}O_2$

Flowable	CAS No.	Formula
1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a,7-trimethyl-, (1R,4aS,7R,10aR)-	7715-76-6	$C_{20}H_{30}O_2$
1-Propanol, 2-(2-ethoxypropoxy)-	15764-24-6	$C_8H_{18}O_3$
1-Propene, 1,1,2,3,3,3-hexafluoro-, oxidized, polymd.	69991-67-9	$[CF(CF_3)CF_2O]_x(CF_2O)_y$
2(3H)-Furanone, 5-decyldihydro-	2721-23-5	$C_{14}H_{26}O_2$
2(3H)-Furanone, 5-dodecyldihydro-	730-46-1	$C_{16}H_{30}O_2$
2(3H)-Furanone, dihydro-5-nonyl-	7370-36-7	$C_{13}H_{24}O_2$
2(3H)-Furanone, dihydro-5-undecyl-	7370-42-5	$C_{15}H_{28}O_2$
2-(4,5-Dihydro-4-methyl-4-isopropyl-5-oxo-1H-imidazol-2-yl)-5-methyl-3-pyridinecarboxylic acid monoammonium salt	115136-53-3	$C_{14}H_{17}N_3O_3H_3N$
2,2,3-Trimethylpentane	564-02-3	C_8H_{18}
2,2,4-Trimethylhexane	16747-26-5	C_9H_{20}
2,2,4-Trimethylpentane-1,3-diol monoisobutyrate	25265-77-4	$C_{12}H_{24}O_3$
2,2-Dimethyl-3-oxopropyl dodecanoate	102985-93-3	$C_{17}H_{32}O_3$
2,3 Dimethyloctane	7146-60-3	$C_{10}H_{22}$
2,3-Dimethylhexane	584-94-1	C_8H_{18}
2,4,7,9-Tetramethyldecane-4,7-diol	17913-76-7	$C_{14}H_{30}O_2$
2,4-D 2-butoxymethylethyl ester	1320-18-9	$C_{15}H_{20}Cl_2O_4$
2,4-D, polypropoxybutyl ester	53467-11-1	$(C_3H_6O)_nC_{12}H_{14}Cl_2O_3$
2,4-D, salts and esters	-	$Cl_2C_6H_3OCH_2CO_2H$
2,5-Furandione, dihydro-, mono-C15-20-alkenyl derivs.	68784-12-3	$C_{22}H_{38}O_3$
20,29,30-Trinorlup-13(18)-ene, (17.alpha.)-	63543-60-2	$C_{27}H_{44}$
20,29,30-Trinorlupane, (17.alpha.)-	55199-72-9	$C_{27}H_{46}$
2-Butene, 1,1,4,4-tetramethoxy-	5370-08-1	$C_8H_{16}O_4$
2-Butenedioic acid (2E)-, di-C12-18-alkyl esters	68921-51-7	$C_{34}H_{64}O_4$
2-Butenedioic acid (2E)-, di-C18-22-alkyl esters	68921-53-9	$C_{40}H_{76}O_4$
2-Chloro-3-methyl-4-(methylsulfonyl)benzoic acid	106904-09-0	$C_9H_9ClO_4S$
2-Chloro-4-tert-amylphenol	5323-65-9	$C_{11}H_{15}ClO$
2-Ethyl-4-(2,2,3-trimethylcyclopent-3-en-1-yl)but-2-en-1-ol	106185-75-5	$C_{14}H_{24}O$
2-Furancarboxaldehyde, (hydroxymethyl)-	25376-49-2	$C_6H_6O_3$
2-Methoxyethyl oleate	111-10-4	$C_{21}H_{40}O_3$
2-Methyl-1-heptanol	60435-70-3	$C_8H_{18}O$
2-Methyl-3,5-dinitrophenol	497-56-3	$C_7H_6N_2O_5$
2-Norpinene-2-ethanol, 6,6-dimethyl-, acetate	35836-72-7	$C_{13}H_{20}O_2$
2-O-alpha-D-Glucopyranosyl-L-ascorbic acid	129499-78-1	$C_{12}H_{18}O_{11}$
2-Oxetanone, 3-C12-16-alkyl-4-C13-17-alkylidene derivs.	84989-41-3	$C_{32}H_{60}O_2$
2-Pentene, 4,4-dimethyl-, (E)-	690-08-4	C_7H_{14}
2-Pentene, 4-methyl-, (E)-	674-76-0	C_6H_{12}
2-Propenal, 3-(4-hydroxy-3,5-dimethoxyphenyl)-	87345-53-7	$C_{11}H_{12}O_4$
2-Propenal, 3-(4-hydroxy-3,5-dimethoxyphenyl)-, (2E)-	4206-58-0	$C_{11}H_{12}O_4$
2-Propenoic acid, 2-hydroxy-1-methylethyl ester	2918-23-2	$C_6H_{10}O_3$
2-Propenoic acid, 2-propylheptyl ester	149021-58-9	$C_{13}H_{24}O_2$

Flowable	CAS No.	Formula
2-Propoxyethanol acetate	20706-25-6	$C_7H_{14}O_3$
3-(Hexyloxy)propane-1,2-diol	10305-38-1	$C_9H_{20}O_3$
3,3'-[Methylenebis(oxymethylene)]bisheptane	22174-70-5	$C_{17}H_{36}O_2$
3,3-Dimethyl-1-Butyne	917-92-0	C_6H_{10}
3,4,6-Trichlorocatechol	32139-72-3	$C_6H_3Cl_3O_2$
3,5,5-Trimethylcyclohex-3-en-1-one	471-01-2	$C_9H_{14}O$
3,5-Dimethyl-1,2-dioxolane-3,5-diol	13784-51-5	$C_5H_{10}O_4$
3-Formylbut-2-enyl acetate	26586-02-7	$C_7H_{10}O_3$
3-Heptene, (3Z)-	7642-10-6	C_7H_{14}
3-O-Ethyl-L-ascorbic acid	86404-04-8	$C_8H_{12}O_6$
4-Butylresorcinol	18979-61-8	$C_{10}H_{14}O_2$
4-Methyl-6-(2,4,4-trimethylpentyl)-2H-pyran-2-one	50650-75-4	$C_{14}H_{22}O_2$
4-Propyl-4'-vinyl-1,1'-bi(cyclohexane)	116020-44-1	$C_{17}H_{30}$
5-(Methoxymethyl)-2-furaldehyde	1917-64-2	$C_7H_8O_3$
6,8-Dimethylnona-3,5-dien-2-one	70214-76-5	$C_{11}H_{18}O$
6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, (5S,6E)-	1937-54-8	$C_{13}H_{22}O$
8-ethylidene-tetracyclo[4.4.0.1(2,5).1(7,10)]dodeca-3-ene	38233-76-0	$C_{14}H_{18}$
8-Quinolinecarboxylic acid, 3,7-dichloro-, compd. with N-methylmethanamine (1:1)	84087-48-9	$C_{10}H_5Cl_2NO_2 \cdot C_2H_7N$
9,10-Epoxystearic acid	2443-39-2	$C_{18}H_{34}O_3$
Abamectin	71751-41-2	$C_{48}H_{72}O_{14}$
Acetates, branched alkyl C7-9 C-8-rich	108419-32-5	$C_{10}H_{18}O_3$
Acetic acid, C8-10-branched alkyl esters, C9-rich	108419-33-6	$C_{11}H_{22}O_2$
Acetic acid, C9-11-branched alkyl esters, C10-rich	108419-34-7	$C_{12}H_{24}O_2$
Aflatoxins	1402-68-2	$C_{17}H_{14}O_6 \cdot C_{17}H_{14}O_7 \cdot C_{17}H_{12}O_6 \cdot C_{17}H_{12}O_7$
Alcohols, C11-14-iso-, C13-rich	68526-86-3	$C_{13}H_{28}O$
Alcohols, C16-18 and C18-unsatd., ethoxylated	68920-66-1	$C_{20}H_{40}O$
Alcohols, C6-12	68603-15-6	$C_6H_{14}O$
Alcohols, ethoxylated C12-14	68439-50-9	$C_{14}H_{30}O$
Aldehydes, C5	-	$C_5H_{10}O$
Aldehydes, C6	-	$C_6H_{12}O$
Alkane sulfonic acids sodium salts	68608-15-1	$C_{14}H_{30}O_3S?Na$
Alkanes, C12-14-iso-	68551-19-9	$C_{13}H_{28}$
Alkenes, c10-13	85535-87-1	$C_{11}H_{22}$
Alkenes, C15-18	93762-80-2	$C_{16}H_{30}$
Allyl 2-hydroxyisobutyrate	19444-21-4	$C_7H_{12}O_3$
Allyl acetoacetate	1118-84-9	$C_7H_{10}O_3$
Amines	-	R-NH2
Ammonium lignosulfonate	8061-53-8	$C_6H_9Cl_2N_7O$
Amprolium	121-25-5	$C_{14}H_{19}N_4 \cdot Cl$
A'-Neo-22,29,30-trinorgammacer-17(21)-ene	65132-06-1	$C_{27}H_{44}$
A'-Neo-22,29,30-trinorgammacerane, (17.alpha.)-	53584-59-1	$C_{27}H_{46}$

Flowable	CAS No.	Formula
A'-Neo-25,28,30-trinorgammacerane, (17.alpha.,21.beta.)-	89675-51-4	$C_{27}H_{46}$
A'-Neo-28,30-dinorgammacerane, (17.alpha.)-	65636-26-2	$C_{28}H_{48}$
A'-Neo-28,30-dinorgammacerane, 17-methyl-, (17.alpha.)-	119613-71-7	$C_{29}H_{50}$
A'-Neo-30-norgammacerane, (17.alpha.)-	53584-60-4	$C_{29}H_{50}$
A'-Neo-30-norgammacerane, (21.beta.)-	3258-87-5	$C_{29}H_{50}$
A'-Neogammacerane	471-62-5	$C_{30}H_{52}$
A'-Neogammacerane, (17.alpha.)-	13849-96-2	$C_{30}H_{52}$
A'-Neogammacerane, (21.beta.)-	1176-44-9	$C_{30}H_{52}$
Alkenes, C10 internal- [19]	-	$C_{10}H_{20}$
Alkenes, C11 internal- [19]	-	$C_{11}H_{22}$
Alkenes, C12 internal- [19]	-	$C_{12}H_{24}$
Antimycin A	1397-94-0	$C_{28}H_{40}N_2O_9$
ar,ar'-Dimethoxybenzidine	1331-53-9	$C_{14}H_{16}N_2O_2$
Aroclor 1268	11100-14-4	$C_{10}H_8O_4$
Aromatics, C10 [20]	-	$C_{10}H_{14}$
Aromatics, C11 [20]	-	$C_{11}H_{16}$
Aromatics, C12 [20]	-	$C_{12}H_{18}$
Aromatics, C9 [20]	-	C_9H_{12}
Benzaldehyde, hydroxy-	28777-87-9	$C_7H_6O_2$
Benzalkonium chloride	8001-54-5	$C_6H_5CH_2N(CH_3)2RCl$ ($R=C_8H_{17}$ to $C_{18}H_{37}$)
Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	68411-46-1	$C_{16}H_{19}N$ - $C_{28}H_{43}N$
Benzene, 1,1'-ethylidenebis-, isopropylated, distn. residues	211578-04-0	$C_{14}H_{14}$
Benzene, 1,3-dipropyl-	17171-72-1	$C_{12}H_{18}$
Benzene, 1-ethyl-2,3,4-trimethyl-	61827-86-9	$C_{11}H_{16}$
Benzene, 1-methyl-4-pentyl-	1595-09-1	$C_{12}H_{18}$
Benzene, alkyl derivs. C10-16	68648-87-3	$C_{18}H_{30}$
Benzene, C10-13-alkyl derivs.	67774-74-7	$C_{16}H_{26}$
Benzene, dialkyl derivs. C11	-	$C_{17}H_{38}$
Benzene, dialkyl derivs. C12	-	$C_{18}H_{30}$
Benzenediol, ethenyl-	104618-88-4	$C_8H_8O_2$
Benzenediol, methyl-	80934-44-7	$C_7H_8O_2$
Benzenemethanol, ar,ar-dimethyl-	29718-36-3	$C_9H_{12}O$
Benzenesulfonic acid, alkyl derivs. C10-13, sodium salts	68411-30-3	$C_6H_5NaO_3S$
Benzofluoranthene	56832-73-6	$C_{20}H_{12}$
Benzoic acid, 4-hydroxy-, methyl and propyl esters	-	$C_{11}H_{14}O_3$
Benzoic acids	-	$C_7H_6O_2$
Benzonaphthothiophene	61523-34-0	$C_{16}H_{10}S$
Bis(2-ethylhexyl) carbonate	14858-73-2	$C_{17}H_{34}O_3$
Bis(2-ethylhexyl) cyclohexane-1,4-dicarboxylate	84731-70-4	$C_{24}H_{44}O_4$
Bis(7-methyloctyl) Cyclohexane-1,2-dicarboxylate	166412-78-8	$C_{26}H_{48}O_4$
Bis-ethoxydiglycol cyclohexane 1,4-dicarboxylate	922165-31-9	$C_{20}H_{36}O_8$

Flowable	CAS No.	Formula
Bis-propylheptyl carbonate	1238449-42-7	$C_{21}H_{42}O_3$
Branched and linear heptyl nonyl phthalate	111381-89-6	$C_{24}H_{38}O_4$
Branched p-nonylphenol	84852-15-3	$C_{15}H_{24}O$
Bufencarb	8065-36-9	$C_{13}H_{19}NO_2 \cdot C_{13}H_{19}NO_2$
Bulan mixt. with 2-nitro-1,1-bis(p-chlorophenyl)propane	8027-00-7	$C_{16}H_{15}Cl_2NO_2 \cdot C_{15}H_{13}Cl_2NO_2$
Butanediol	25265-75-2	$HOCH_2CH_2CH_2CH_2OH$
Butene	25167-67-3	C_4H_8
Butoxypolypropylene glycol	9003-13-8	$(C_3H_6O)_nC_4H_{10}O$
Butylbenzene isomers [21]	-	$C_{10}H_{14}$
C.I. Acid Yellow 3	8004-92-0	$C_{18}H_9NO_8S_2Na$
C10-rich C9-11 Alkenes	68526-56-7	$C_{10}H_{16}$
C12-14-Alkyldimethyl(ethylbenzyl) ammonium chlorides	85409-23-0	$C_{23}H_{42}ClN$
C12-18-Alkyldimethylbenzyl ammonium chlorides	68391-01-5	$C_{23}H_{42}ClN$
C13-Rich C11-14-branched alkyl acetates	108419-35-8	$C_{15}H_{30}O_2$
C18-Unsatd. fatty acids dimers	61788-89-4	$C_{36}H_{64}O_4$
C3-4-Hydrocarbons	68476-40-4	C_4H_{10}
C5 alkenes	68527-11-7	C_5H_{10}
C6 alkenes	68526-52-3	C_6H_{12}
C8-18 and C18-Unsaturated fatty acids ammonium salts [22]	84776-33-0	$C_9H_{17}O_2^-(NH_4)^+$
Caliche	-	$CaCO_3$
Carbamodithioic acid(l)	4384-82-1	CH_2NS_2
Carbamodithioic acid, cyano-, disodium salt, mixt. with 1,2-ethanediamine and methylcarbamodithioic acid monopotassium salt	8070-47-1	$C_6H_{17}KN_5NaS_4$
Carbon black	1333-86-4	C
Carbonodithioic acid, O-butyl ester	110-50-9	$C_5H_{10}OS_2$
Carboxylic acids, C5-9, hexaesters with dipentaerythritol	67762-52-1	$C_{10}H_{22}O_7 \cdot$ Unspecified
Carboxylic acids, C5-9, tetraesters with pentaerythritol	67762-53-2	$C_{33}H_{68}O_4$
Carboxylic acids, di-, C4-6	68603-87-2	$C_2H_2O_4$
Castor oil	8001-79-4	$C_{57}H_{104}O_9$
Chitosan	9012-76-4	$(C_6H_{11}NO_4)_n$
Chlordane, technical	12789-03-06	$C_{10}H_6Cl_8$
Chlorinated phenols	1336-35-2	C[Cl]
Chlorobenzoic acid	26264-09-5	$C_7H_5ClO_2$
Chlorohexane	25495-90-3	$C_6H_{13}Cl$
Chloronaphthalene	25586-43-0	$C_{10}H_7Cl$
Chlorophenol	25167-80-0	C_6H_5ClO
Chlorophyll c	11003-45-5	$C_{35}H_{30}MgN_4O_5$
Chlorotetrafluoroethane	63938-10-3	C_2HClF_4
Cholestane, (5.alpha.,14.beta.,20S)-	69483-48-3	$C_{27}H_{48}$
cis-2-Hexene	7688-21-3	C_6H_{12}
Clam-trol CT 1	126851-28-3	$C_{24}H_{16}BrN$

Flowable	CAS No.	Formula
Clove oil [23]	8000-34-8	$C_7H_{12}ClN_3O_2$
Cobalt 2-ethylhexanoate	13586-82-8	$C_8H_{16}O_2 \cdot xCo$
Cobalt carbonate	7542-09-8	$CH_2O_3 \cdot xCo$
Cobalt hydrocarbonyl	16842-03-8	C_4HCoO_4
Cobalt naphthenate	61789-51-3	$2(C_{11}H_7O_2) \cdot Co$
Cocamides diethanolamines	68603-42-9	$C_{13}H_{13}Cl_8NO_4$
Coco amides	8051-30-7	$C_4H_{11}NO_2 \cdot$ Unspecified
Copper, bis(acetato-.kappa.O)diammine-	13822-80-5	$C_4H_{12}CuN_2O_4$
Cumylphenyl diphenyl phosphate	34364-42-6	$C_{27}H_{25}O_4P$
Cyanate	661-20-1	CNO
Cyanide compounds	-	CN-X
Cyclohexane, 1,1,3,4-tetramethyl-	24612-75-7	$C_{10}H_{20}$
Cyclohexane, 1,2,4-trimethyl-, (1.alpha.,2.alpha.,4.alpha.)-	1678-80-4	C_9H_{18}
Cyclohexane, 1,2,4-trimethyl-, (1R,2R,4R)-rel-	7667-60-9	C_9H_{18}
Cyclohexane, 1,2,4-trimethyl-, (1R,2S,4R)-rel-	7667-58-5	C_9H_{18}
Cyclohexane, 1,2-diethyl-1-methyl-	61141-79-5	$C_{11}H_{22}$
Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.beta.)-	1795-26-2	C_9H_{18}
Cyclohexane, 1-ethyl-1,2-dimethyl-	824-01-1	$C_{10}H_{20}$
Cyclohexane, 1-ethyl-2,3-dimethyl-	7058-05-1	$C_{10}H_{20}$
Cyclohexane, 1-ethyl-2,4-dimethyl-	61142-69-6	$C_{10}H_{20}$
Cyclohexane, 1-ethyl-3-methyl-, (1R,3R)-rel-	4926-76-5	C_9H_{18}
Cyclohexane, 1-methyl-2-(1-methylethyl)-	16580-23-7	$C_{10}H_{20}$
Cyclohexane, 1-methyl-3-(1-methylethyl)-	16580-24-8	$C_{10}H_{20}$
Cyclohexane, 1-propenyl-	5364-83-0	C_9H_{16}
Cyclohexane, diethylmethyl-	82162-00-3	$C_{11}H_{22}$
Cyclohexane, dimethyl(methylpropyl)-	88456-07-9	$C_{12}H_{24}$
Cyclohexane, ethyldimethyl-	31902-94-0	$C_{10}H_{20}$
Cyclohexane, ethylpropyl-	211180-47-1	$C_{11}H_{22}$
Cyclohexane, heneicosyl-	26718-82-1	$C_{27}H_{54}$
Cyclohexane, methyl(1-methylethyl)-	52993-54-1	$C_{10}H_{20}$
Cyclohexane, pentylidene-	39546-79-7	$C_{11}H_{20}$
Cyclohexylglycerin	10305-41-6	$C_9H_{18}O_3$
Cyclopentane, 1,2,3-trimethyl-, (1.alpha.,2.alpha.,3.beta.)-	15890-40-1	C_8H_{16}
Cyclopentane, 1,2,4-trimethyl-, (1.alpha.,2.beta.,4.alpha.)-	16883-48-0	C_8H_{16}
Cyclopentane, 1-ethyl-3-methyl-	3726-47-4	C_8H_{16}
Cyclopentane, tetramethyl-	67784-41-2	C_9H_{18}
Cyclopentene, 1-methyl-	693-89-0	C_6H_{10}
Cyclopentene, 3-methyl-	1120-62-3	C_6H_{10}
Cyclopentenone, trimethyl-	86368-24-3	$C_8H_{12}O$
Cyclopropylacetylene	6746-94-7	C_5H_6
Decane, 2,7-dimethyl-	17312-51-5	$C_{12}H_{26}$
Decane, 4,5-dimethyl-	17312-46-8	$C_{12}H_{26}$

Flowable	CAS No.	Formula
Decane, 4-ethyl-	1636-44-8	$C_{12}H_{26}$
Decane, dimethyl-	36473-07-1	$C_{12}H_{26}$
Decene	25339-53-1	$C_{10}H_{20}$
Decene, methyl-	73752-14-4	$C_{11}H_{22}$
Demeton	8065-48-3	$C_8H_{19}O_3PS_2 \cdot C_8H_{19}O_3PS_2$
Demeton-methyl	8022-00-2	$C_6H_{15}O_3PS_2 \cdot C_6H_{15}O_3PS_2$
Diamond	7782-40-3	C
Dicamba N,N-bis(3-aminopropyl)methylamine salt	1286239-22-2	$C_{15}H_{25}Cl_2N_3O_5$
Dichlorobenzotrifluoride	30498-35-2	$C_7H_3Cl_2F_3$
Dichloroethane	1300-21-6	$C_2H_4Cl_2$
Dichloroethylene	25323-30-2	$C_2H_2Cl_2$
Dichloropentafluoropropane	127564-92-5	$C_3HCl_2F_5$
Dichlorophenol	25167-81-1	$C_6H_4Cl_2O$
Dichloropropane	26638-19-7	$C_3H_6Cl_2$
Dichloropropene	26952-23-8	$C_3H_4Cl_2$
Dichlorotoluene	29797-40-8	$C_7H_6Cl_2$
Dichlorotrifluoroethane	34077-87-7	$C_2HCl_2F_3$
Dichlorprop isooctyl ester	28631-35-8	$C_{17}H_{24}Cl_2O_3$
Didodecyl fumarate	2402-58-6	$C_{28}H_{52}O_4$
Diethyl 1,2-cyclopentanedicarboxylate	90474-13-8	$C_{11}H_{18}O_4$
Diethyl 2-(2-oxopropyl)succinate	1187-74-2	$C_{11}H_{18}O_5$
Diethylbenzene	25340-17-4	$C_{10}H_{14}$
Diethylene glycol diglycidyl ether	4206-61-5	$C_{10}H_{18}O_5$
Diethylene glycol mono-2-cyanoethyl ether	10143-54-1	$C_7H_{13}NO_3$
Diethylene glycol mono-2-methylpentyl ether	10143-56-3	$C_{10}H_{22}O_3$
Diisooctyl phthalate	27554-26-3	$C_{24}H_{38}O_4$
Diisopropylnaphthalene	38640-62-9	$C_{16}H_{20}$
Dimethylphenanthrene	29062-98-4	$C_{16}H_{14}$
Dimethylphenol	1300-71-6	$C_8H_{10}O$
Dinitrophenol	25550-58-7	$C_6H_4N_2O_5$
Dinocap	39300-45-3	$C_{18}H_{24}N_2O_6$
Dipropylene glycol	25265-71-8	$C_6H_{14}O_3$
Dipropylene glycol monomethyl ether	34590-94-8	$C_7H_{16}O_3$
Dipropyleneglycol methyl ether acetate	88917-22-0	$C_9H_{18}O_4$
Disodium dodecyl(sulphonatophenoxy)benzenesulphonate	28519-02-0	$C_{24}H_{34}O_7S_2 \cdot 2Na$
Dissolved Organic Carbon	-	C
Ditetradecyl fumarate	10341-03-4	$C_{32}H_{60}O_4$
Dodecenal	82107-89-9	$C_{12}H_{22}O$
Dodecene	25378-22-7	$C_{12}H_{24}$
Dodecylguanidine	112-65-2	$C_{13}H_{29}N_3$
Emamectin benzoate	155569-91-8	$C_7H_6O_2 \cdot$ Unspecified
Enovid	8015-30-3	$C_{20}H_{26}O_2$
Eprinomectin	123997-26-2	$C_{50}H_{75}NO_{14}$
Ergostane	25318-39-2	$C_{28}H_{50}$
Ethane, 1,1,1,2,2-pentafluoro-2-methoxy-	22410-44-2	$C_3H_3F_5O$

Flowable	CAS No.	Formula
Ethane, 1,1,1,2-tetrafluoro-2-(trifluoromethoxy)-	2356-62-9	C_3HF_7O
Ethane, 1,1-difluoro-2-(trifluoromethoxy)-	84011-15-4	$C_3H_3F_5O$
Ethane, 2-(difluoromethoxy)-1,1,1,2-tetrafluoro-, (+-)-	57041-67-5	$C_3H_2F_6O$
Ethanes, chlorinated	68411-72-3	C_2H_5Cl
Ethanone, 1-phenyl-, monohydroxy deriv.	41903-50-8	$C_8H_8O_2$
Ethenylphenol	31257-96-2	C_8H_8O
Ethyl cellulose	9004-57-3	$C_2H_6O \cdot x\text{Unspecified}$
Ethylene glycol bis(2,3-epoxy-2-methylpropyl) ether	3775-85-7	$C_{10}H_{18}O_4$
Ethylene glycol diacetoacetate	5459-04-1	$C_{10}H_{14}O_6$
Ethylene glycol mono-2,4-hexadienyl ether	27310-21-0	$C_8H_{14}O_2$
Ethylene glycol mono-2-methylpentyl ether	10137-96-9	$C_8H_{18}O_2$
Ethylene glycol mono-sec-butyl ether	7795-91-7	$C_6H_{14}O_2$
Ethylenediaminetetraacetic acid ammonium salt	7379-26-2	$C_{10}H_{16}N_2O_8 \cdot xH_3N$
Ethyltoluene	25550-14-5	C_9H_{12}
Fatty acids	67254-79-9	$C_4H_8O_2$
Fatty acids, C14-22	68424-37-3	$C_{17}H_{34}O_2$
Fatty acids, C16-18	67701-03-5	$C_{17}H_{34}O_2$
Fatty acids, C16-18, esters with ethylene glycol	91031-31-1	$C_{36}H_{70}O_5$
Fatty acids, C8-10, C12-18-alkyl esters	95912-86-0	$C_{42}H_{84}O_4$
Fatty acids, C9-13-neo-	68938-07-8	$C_{12}H_{24}O_2$
Fenchyl acetate	4057-31-2	$C_{12}H_{20}O_2$
Ferricyanide	13408-62-3	C_6FeN_6
Fluoranthene, methyl-	30997-39-8	$C_{17}H_{12}$
Fluorenes, C2	-	$C_{13}H_{10}$
Fuller's earth	8031-18-3	$C_{19}H_{17}N_3O_4S_2$
Garlic oil	8000-78-0	$C_{18}H_{32}OS_7$
Gibberellin A4 mixture with Gibberellin A7	8030-53-3	$C_{19}H_{24}O_5 \cdot C_{19}H_{22}O_5$
Glycerides, C12-18	67701-26-2	$C_{15}H_{30}O_4$
Glycerides, C14-18	67701-27-3	$C_{16}H_{32}O_4$
Glycerides, C16-18 mono- and di-	85251-77-0	$C_{37}H_{72}O_5$
Glycerides, C16-22	68002-70-0	$C_{19}H_{38}O_4$
Glycerol octanoate decanoate	65381-09-1	$C_{10}H_{20}O_2 \cdot xC_8H_{16}O_2 \cdot xC_3H_8O_3$
Glyceryl behenate	77538-19-3	$C_{25}H_{50}O_4$
Glycidyl neodecanoate	26761-45-5	$C_{13}H_{24}O_3$
Gold cyanide	37187-64-7	CAuN
Guazatine	108173-90-6	$C_{18}H_{41}N_7$
HCFC-131	359-28-4	$C_2H_2Cl_3F$
HCFC-132	431-06-1	$C_2H_2Cl_2F_2$
HCFC-231bb	421-94-3	$C_3H_2Cl_5F$
HCFC-233fb	7125-84-0	$C_3H_2Cl_3F_3$
HCFC-234ba	425-94-5	$C_3H_2Cl_2F_4$
HCFC-241db	666-27-3	$C_3H_3Cl_4F$
HCFC-244	134190-50-4	$C_3H_3ClF_4$
HCFC-251dc	421-41-0	$C_3H_4Cl_3F$
HCFC-253	134237-44-8	$C_3H_4F_3Cl$

Flowable	CAS No.	Formula
HCFC-261ba	420-97-3	$C_3H_5Cl_2F$
HCFC-262	134190-53-7	$C_3H_5ClF_2$
HCFC-271fb	430-55-7	C_3H_6ClF
Heptachloro-2-norbornene	28680-45-7	$C_7H_3Cl_7$
Heptachlorobiphenyl	28655-71-2	$C_{12}H_3Cl_7$
Heptachlorodibenzofuran	38998-75-3	$C_{12}HCl_7O$
Heptachlorodibenzo-p-dioxin	37871-00-4	$C_{12}HCl_7O_2$
Heptane, 2,2,4-trimethyl-	14720-74-2	$C_{10}H_{22}$
Heptane, 2,2,5-trimethyl-	20291-95-6	$C_{10}H_{22}$
Heptane, 2,5-dimethyl-	2216-30-0	C_9H_{20}
Heptane, dimethyl-	30498-66-9	C_9H_{20}
Heptene	25339-56-4	C_7H_{14}
Hexabromocyclododecane	25637-99-4	$C_{12}H_{18}Br_6$
Hexachlorobiphenyl	26601-64-9	$C_{12}H_4Cl_6$
Hexachlorocyclohexane	27154-44-5	$C_6H_6Cl_6$
Hexachlorodibenzofuran	55684-94-1	$C_{12}H_2Cl_6O$
Hexachlorodibenzo-p-dioxin	34465-46-8	$C_{12}H_2Cl_6O_2$
Hexane, 2,3,5-trimethyl-	1069-53-0	C_9H_{20}
Hexane, ethylmethyl-	79004-87-8	C_9H_{20}
Hexanedioic acid, 2,2,4 (or 2,4,4)-trimethyl-	53445-37-7	$C_9H_{16}O_4$
Hexene	25264-93-1	C_6H_{12}
Hexene, trimethyl-	95461-54-4	C_9H_{18}
HFC-1234ze(E)	1645-83-6	$C_3H_2F_4$
HFC-236cb	677-56-5	$C_3H_2F_6$
HFE 7100	219484-64-7	$C_{10}H_6F_{18}O_2$
HFE-329mcc2	134769-21-4	C_4HF_9O
HFE-338pcc13 (HG-01)	188690-78-0	$C_4H_2F_8O_2$
HFE-347mcf2	171182-95-9	$C_4H_3F_7O$
HFE-356mec3	382-34-3	$C_4H_4F_6O$
HFE-356pcf2	50807-77-7	$C_4H_4F_6O$
Hi-Sol 10	64427-33-4	$C_{72}H_{129}NO$
Hydrocarbons, C14-30, olefin-rich	68514-35-2	$C_{26}H_{42}$
Hydrocarbons, C3	68606-26-8	C_3H_6
Hydrocarbons, c4, 1,3-butadiene-free, polymd., dibutylene fraction	91052-99-2	C_8H_{16}
Hydrocarbons, c4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated	93685-78-0	$C_{16}H_{34}$
Hydrocarbons, C4, 1,3-butadiene-free, polymd., pentaisobutylene fraction, hydrogenated	93685-79-1	$C_{20}H_{42}$
Hydrocarbons, c4, 1,3-butadiene-free, polymd., triisobutylene fraction	91053-01-9	$C_{12}H_{24}$
Hydrocarbons, C4-10-unsatd.	68514-38-5	C_6H_{10}
Hydrocarbons, C4-6, C5-rich	68476-43-7	C_5H_{12}
Hydrocarbons, C5-rich	68476-55-1	C_5H_{12}
Hydrogenated castor oil	8001-78-3	$C_{57}H_{110}O_9$
Hydrogenated terphenyl	61788-32-7	$C_{18}H_{22}$

Flowable	CAS No.	Formula
Imazamethabenz-methyl	81405-85-8	$C_{16}H_{20}N_2O_3$
Isodecanol	25339-17-7	$C_{10}H_{22}O$
Isononanol	27458-94-2	$C_9H_{20}O$
Isooctadecanol	27458-93-1	$C_{18}H_{38}O$
Isooctane	26635-64-3	C_8H_{18}
Isooctanol	26952-21-6	$C_8H_{18}O$
Isopropylbiphenyl	25640-78-2	$C_{15}H_{16}$
Isosorbide dicaprylate	64896-70-4	$C_{22}H_{38}O_6$
Isostearyl palmitate	72576-80-8	$C_{34}H_{68}O_2$
Isotridecanol	27458-92-0	$C_{13}H_{28}O$
Ivermectin	70288-86-7	$C_{48}H_{74}O_{14}$
Jojoba wax [24]	61789-91-1	$CH_3(CH_2)_7CH = CH\text{-}(CH_2)_7CO\text{-}O\text{-}(CH_2)_{11}CH = CH(CH_2)_7CH_3$
Laminaran	9008-22-4	$C_{18}H_{32}O_{16}$
Lead naphthenate	61790-14-5	$C_{22}H_{14}O_4Pb$
Lead stearate	7428-48-0	$C_{18}H_{36}O_2 \cdot xPb$
Lecithins	8002-43-5	$C_{42}H_{80}NO_8P$
Light aromatic solvent naphtha (petroleum)	64742-95-6	C6H6-C4H11
Lignosulfonic acid	8062-15-5	$C_{20}H_{26}O_{10}S_2$
Mancozeb	8018-01-7	$C_4H_6MnN_2S_4 \cdot C_4H_6N_2S_4Zn$
Manganese cyclopentadienyl tricarbonyl	12079-65-1	$C_8H_5MnO_3$
Manganese naphthenate	1336-93-2	$C_{22}H_{14}MnO_4$
MCPA-isooctyl	26544-20-7	$C_{17}H_{25}ClO_3$
m-Cresol compd. with p-cresol (2:1)	15831-10-4	$C_7H_8O \cdot \frac{1}{2} C_7H_8O$
m-Cresol, p-cresol, formaldehyde polymer	27029-76-1	$(C_7H_8O \cdot C_7H_8O \cdot CH_2O)_x$
Mercury, [.mu.-[[3,3'-methylenebis[2-naphthalenesulfonato-.kappa.O]](2-)]]diphenyldi-	14235-86-0	$C_{33}H_{24}Hg_2O_6S_2$
Methacrylic acid homopolymer	25087-26-7	$(C_4H_6O_2)_x$
methyl (1R,2S)-3-oxo-2-pentylcyclopentane-1-carboxylate	1271488-66-4	$C_{12}H_{10}O_3$
Methyl 3-Methoxyacrylate	5788-17-0	$C_5H_8O_3$
Methyl cellosolve acetyl ricinoleate	140-05-6	$C_{23}H_{42}O_5$
Methylanthracene	26914-18-1	$C_{15}H_{12}$
Methylbenzaldehyde	1334-78-7	C_8H_8O
Methylbenzopyrene	65357-69-9	$C_{21}H_{18}$
Methylchrysene	41637-90-5	$C_{19}H_{14}$
Methylfluorene	26914-17-0	$C_{14}H_{12}$
Methylphenanthrene	31711-53-2	$C_{15}H_{12}$
Metiram	9006-42-2	$(C_{16}H_{33}N_{11}S_{16}Zn_3)_x$
Mevinphos	7786-34-7	$C_7H_{13}O_6P$
Naphthalene, 1-ethyl-2-methyl-	17057-93-1	$C_{13}H_{14}$
Naphthalene, 2-ethyl-1-methyl-	25607-16-3	$C_{13}H_{14}$
Naphthalene, decahydromethyl-	28258-89-1	$C_{11}H_{20}$
Naphthalene, dihydro-	29828-28-2	$C_{10}H_{10}$
Naphthalenesulfonic acids	68153-01-5	$C_{10}H_8O_3S$
Naphthenic acids	1338-24-5	$C_{10}H_{18}O_2$

Flowable	CAS No.	Formula
Neodecanoic acid, lead salt	27253-28-7	$C_{10}H_{20}O_2 \cdot xPb$
Neononanoic acid	59354-78-8	$C_9H_{18}O_2$
Nickel carbide	12710-36-0	Ni_3C
Nickelate(2-), tetrakis(cyano-.kappa.C)-, dipotassium, (SP-4-1)-	14220-17-8	$C_4N_4Ni \cdot 2K$
N-Isopropyl-2-butanonimine	38836-39-4	$C_7H_{15}N$
Nonachlorobiphenyl	53742-07-7	$C_{12}HCl_9$
Nonadecanedioic acid	6250-70-0	$C_{19}H_{36}O_4$
Nonadiene	71030-52-9	C_9H_{16}
Nonane, 2,6-dimethyl-	17302-28-2	$C_{11}H_{24}$
Nonane, 3,5-dimethyl-	17302-25-9	$C_{11}H_{24}$
Nonane, 3-ethyl-	17302-11-3	$C_{11}H_{24}$
Nonane, 5-(1-methylethyl)-	62184-72-9	$C_{12}H_{26}$
Octachlorobiphenyl	55722-26-4	$C_{12}H_2Cl_8$
Octadecanoic acid, branched and linear	68201-37-6	$C_{18}H_{36}O_2$
Octane, 2,4-dimethyl-	4032-94-4	$C_{10}H_{22}$
Octane, 3-ethyl-3-methyl-	17302-16-8	$C_{11}H_{24}$
Octane, dimethyl-	63335-88-6	$C_{10}H_{22}$
Octane, ethyl-	208038-45-3	$C_{10}H_{22}$
Octene	25377-83-7	C_8H_{16}
Octoxynol 9	9002-93-1	$(C_2H_4O)_nC_{14}H_{22}O$
Octylphenol	67554-50-1	$C_{14}H_{22}O$
Oleyl erucate	17673-56-2	$C_{40}H_{76}O_2$
Oligomeric D-glucopyranose decyl octyl glycosides	68515-73-1	$C_{16}H_{32}O_6$
Organic carbon, PM2.5 LC	-	C
Paraffin, C10 [20]	-	$C_{10}H_{20}$
Paraffin, C11 [20]	-	$C_{11}H_{22}$
Paraffin, C12 [20]	-	$C_{12}H_{24}$
Paraffin, C13 [20]	-	$C_{13}H_{26}$
Paraffin, C7 [20]	-	C_7H_{14}
Paraffin, C8 [20]	-	C_8H_{16}
Paraffin, C9 [20]	-	C_9H_{18}
Pentabromodiphenyl ether	32534-81-9	$C_{12}H_5Br_5O$
Pentachlorobiphenyl	25429-29-2	$C_{12}H_5Cl_5$
Pentachlorodibenzofuran	30402-15-4	$C_{12}H_3Cl_5O$
Pentachlorodibenzo-p-dioxin	36088-22-9	$C_{12}H_3Cl_5O_2$
Pentadecenal	118624-11-6	$C_{15}H_{28}O$
Pentaerythrityl tetraheptanoate	25811-35-2	$C_{33}H_{60}O_8$
Pentaerythrityl tetraisononanoate	93803-89-5	$C_{41}H_{76}O_8$
Pentafluorobutane	141529-32-0	$C_4H_5F_5$
Pentanol isomers	30899-19-5	$C_5H_{12}O$
Pentene, 3-ethyl-	162071-36-5	C_7H_{14}
Perfluorodecalin (cis)	60433-11-6	$C_{10}F_{18}$
Perfluorodecalin (trans)	60433-12-7	$C_{10}F_{18}$
Phenol, (1,1-dimethylethyl)-	27178-34-3	$C_{10}H_{14}O$
Phenol, 2,6-dimethoxy(2-propenyl)-	148425-13-2	$C_{11}H_{14}O_3$

Flowable	CAS No.	Formula
Phenol, 2-methoxymethyl-	29034-41-1	$C_8H_{10}O_2$
Phenol, 4,5-dimethyl-2-(1-methylethyl)-	35786-94-8	$C_{11}H_{16}O$
Phenol, alkyl derivs. C10	-	$C_{10}H_{14}O$
Phenol, alkyl derivs. C11	-	$C_{11}H_{16}O$
Phenol, ethyl-2-methoxy-	29760-89-2	$C_9H_{12}O_2$
Phenol, heptyl derivs.	72624-02-3	$C_{13}H_{20}O$
Phenol, thiobis[tetrapropylene-	68815-67-8	$C_{36}H_{58}O_2S$
Phthalates, branched and linear dialkyl C7-11	68515-42-4	$C_{24}H_{38}O_4$
Phthalates, branched and linear dialkyl C9-11	68515-43-5	$C_{24}H_{38}O_4$
Phthalates, branched dialkyl C11-14, C13-rich	68515-47-9	$C_{31}H_{52}O_4$
Phthalates, branched dialkyl C8-10, C9-rich	68515-48-0	$C_{26}H_{42}O_4$
Phthalates, branched dialkyl C9-11, C10-rich	68515-49-1	$C_{28}H_{46}O_4$
Phthalates, dialkyl C6-10	68515-51-5	$C_{20}H_{30}O_4$+$C_{24}H_{38}O_4$+ $C_{28}H_{46}O_4$
Phthalates, dialkyl C8-10	71662-46-9	$C_{25}H_{40}O_4$
Phthalic acid mixed decyl and lauryl and octyl diesters	70693-30-0	$C_{38}H_{66}O_{10}$
Picrotoxin	124-87-8	$C_{15}H_{18}O_7 \cdot C_{15}H_{16}O_6$
Poly(iminoimidocarbonyliminoimidocarbonyliminohexamethylene) hydrochloride	32289-58-0	$(C_8H_{17}N_5)_n \cdot xHCl$
Polyacrylic acid	9003-01-4	$C_5H_{10}O_2$
Polyethylene glycol	25322-68-3	$H(OCH_2CH_2)_nOH$
Polyethylene glycol mono(branched tridecyl) ether	69011-36-5	$C_{13}H_{28}O$
Polyethylene glycol mono-C12-14-alkyl ether sulfate sodium salt	68891-38-3	$C_{24}H_{50}Na_2O_5S$
Polysorbate 20	9005-64-5	$C_{2n}H_{4n+2}O_{n+1}$
Povidone-iodine	25655-41-8	$C_6H_9NO \cdot I_2$
Propane, 1-bromo-1,1,2,3,3,3-hexafluoro-	2252-78-0	C_3HBrF_6
Propanoic acid, 2-(2,4,5-trichlorophenoxy)-, salts and esters	-	$C_{13}H_{15}Cl_3O_3$
Propanoic acid, 2-hydroxy-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester, (2S)-	61597-98-6	$C_{13}H_{24}O_3$
Propylene glycol monobutyl ether	29387-86-8	$C_7H_{16}O_2$
Propylene glycol monomethyl ether acetate	84540-57-8	$C_6H_{12}O_3$
Propylene glycol monopropyl ether	30136-13-1	$C_6H_{14}O_2$
Propylheptyl caprylate	868839-23-0	$C_{18}H_{36}O_2$
Pyrene, methyl-	27577-90-8	$C_{17}H_{12}$
Pyrene, nitro-	63021-86-3	$C_{16}H_9NO_2$
Pyrethrins	8003-34-7	$C_{43}H_{56}O_8$
Pyridine, 3-[(2S)-1-methyl-1-oxido-2-pyrrolidinyl]-	491-26-9	$C_{10}H_{14}N_2O$
Pyridine, phenyl-	52642-16-7	$C_{11}H_9N$
Pyridinol	27341-45-3	C_5H_5NO
Resin acids [25]	-	$C_{20}H_{30}O_2$
Rhodamine WT	37299-86-8	$C_{29}H_{29}ClN_2Na_2O_5$
Sevoflurane	28523-86-6	$C_4H_3F_7O$
Silvex isooctyl ester	32534-95-5	$C_{17}H_{23}Cl_3O_3$
Sitosterols	12002-39-0	$C_{29}H_{52}O$

Flowable	CAS No.	Formula
Sodium [[(phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]tetrakisphosphonate	22042-96-2	$C_9H_{27}N_3NaO_{15}P_5$
Sodium alizarinesulfonate	130-22-3	$C_{14}H_7NaO_7S$
Sodium lauryl ether sulfate	9004-82-4	$C_{14}H_{29}O_5S \cdot Na$
Sodium lignosulfonate	8061-51-6	$C_{20}H_{24}Na_2O_{10}S_2$
Sodium polyacrylate	9003-04-7	$C_3H_4O_2$
Sodium tridecylbenzenesulfonate	26248-24-8	$C_{19}H_{31}NaO_3S$
Spinetoram	935545-74-7	$C_{42}H_{69}NO_{10}$
Spinosad	168316-95-8	$C_{83}H_{132}N_2O_{20}$
Stigmast-4-en-3-one	1058-61-3	$C_{29}H_{48}O$
Stoddard solvent	8052-41-3	$C_8H_{15}BrO_2$
Strychnidin-10-one, and salts	-	$C_{23}H_{26}N_2O_4$
Syrups, hydrolyzed starch, hydrogenated	68425-17-2	$C_{18}H_{34}O_{16}$
Tannic acid	1401-55-4	$C_{76}H_{52}O_{46}$
Terpenes	129874-8-4	$C_{24}H_{40}O_5$
Terphenyl	26140-60-3	$C_{18}H_{14}$
Terpineol	8000-41-7	$C_{10}H_{18}O$
Tetrachlorobenzene	12408-10-5	$C_6H_2Cl_4$
Tetrachlorobiphenyl	26914-33-0	$C_{12}H_6Cl_4$
Tetrachlorodibenzo-p-dioxin	41903-57-5	$C_{12}H_4Cl_4O_2$
Tetrachloroethane	25322-20-7	$C_2H_2Cl_4$
Tetrachlorophenol	25167-83-3	$C_6H_2Cl_4O$
Tetrachlorotetrafluoropropane	29255-31-0	$C_3Cl_4F_4$
Tetradecanol	27196-00-5	$C_{14}H_{30}O$
Tetramethylbenzene	25619-60-7	$C_{10}H_{14}$
Tetrapropylenebenzenesulfonic acid	11067-81-5	$C_{18}H_{22}O_3S$
Thyme oil [26]	8007-46-3	$C_{50}H_{82}O_4$
Toluene diisocyanate	26471-62-5	$(NCO)_2C_6H_3CH_3$
Toluene-2,5-diamine sulfate	6369-59-1	$C_7H_{12}N_2O_4S$
Toluenediamine	25376-45-8	$2C_7H_{10}N_2$
Toluidine	26915-12-8	C_7H_9N
Total carbon	-	C
Total organic carbon	-	C
Trichlorobenzene	12002-48-1	$C_6H_3Cl_3$
Trichloroethane	25323-89-1	$C_2H_3Cl_3$
Trichloroguaiacol	61966-36-7	$C_7H_5Cl_3O_2$
Trichlorophenol	25167-82-2	$C_6H_3Cl_3O$
Trichloropropane	25735-29-9	$C_3H_5Cl_3$
Trichlorotoluene	30583-33-6	$C_7H_5Cl_3$
Trichlorotrifluoroethane	26523-64-8	$C_2Cl_3F_3$
Tricresyl phosphate	1330-78-5	$(CH_3C_6H_4O)_3PO$
Tridecane, 2,6,10-trimethyl-	3891-99-4	$C_{16}H_{34}$
Triisononanoin	56554-53-1	$C_{30}H_{56}O_6$
Trimedlure	12002-53-8	$C_{12}H_{21}ClO_2$
Trimethylbenzene	25551-13-7	C_9H_{12}
Trimethylhexamethylenediamine	25620-58-0	$C_{18}H_{44}N_4$

Flowable	CAS No.	Formula
Trimethylnaphthalene	28652-77-9	$C_{13}H_{14}$
Turpentine	9005-90-7	$C_{10}H_{16}$
Undecane, 3-methyl-	1002-43-3	$C_{12}H_{26}$
Undecane, 5-methyl-	1632-70-8	$C_{12}H_{26}$
Veratrine (mixture)	8051-02-3	$C_{32}H_{49}NO_9$
Vinyl neodecanoate	51000-52-3	$C_{12}H_{22}O_2$
Xanthacridinum	8048-52-0	$C_{14}H_{14}ClN_3$
Zinc bis(O,O-diisooctyl dithiophosphate)	28629-66-5	$C_{32}H_{68}O_4P_2S_4Zn$

Appendix B: Complex Molecular Formulas

Many flowables in FEDEFL are not discrete structures and are instead mixtures or groups. **Exhibit B-1** catalogues the carbon contents assigned to these complex flows. Documentation on flow composition and calculation steps are included in the accompanying calculations workbook.

Exhibit B-1. Carbon Content of Complex Flows

Flowable	CAS No.	Carbon Content (kg C/kg)	Comments
Acid compounds	-	0.2857	Source: [11, 27]. Calculated as an average of 168 carboxylic, strong (oxidizing and non-oxidizing), and weak acids.
Acids, volatile	-	0.5666	Source: [28]. Calculated as an average of 7 volatile acids.
Air	132259-10-0	1.094E-06	Source: [29]. Assumes average air composition with a water vapor content of 2%. The water vapor content of the atmosphere can range from 0% to 4%, but this changes the carbon content by less than 0.005%.
Alcohols	-	0.5380	Source: [11]. Calculated as an average of 350 alcohols.
Aliphatics	-	0.8529	Source: [30, 31]. Calculated as an average of 104 aliphatics.
Ammonium compounds, quarternary	-	0.7210	Source: [32]. Calculated as an average of 24 QACs.
Anesthetics	-	0.4283	Source: [33]. Calculated as an average of 20 inhalation and intravenous general anesthetics.
Aroclor 1016	12674-11-2	0.5557	Source: [34]
Aroclor 1221	11104-28-2	0.7089	Source: [34]
Aroclor 1232	11141-16-5	0.6205	Source: [34]
Aroclor 1242	53469-21-9	0.5381	Source: [34]
Aroclor 1248	12672-29-6	0.4863	Source: [34]
Aroclor 1254	11097-69-1	0.4355	Source: [34]
Aroclor 1260	11096-82-5	0.3847	Source: [34]
Aroclor 1262	37324-23-5	0.3730	Source: [34]
Aromatic hydrocarbons	63231-51-6	0.9209	Source: [31]. Assume same as polycyclic aromatic hydrocarbons.
Aromatics	-	0.7759	Source: [11]. Calculated as an average of 217 aromatics.
Aromatics, purgeable	-	0.6930	Source: [35]. Calculated as an average of 7 purgeable aromatics.
Aromatics, substituted	-	0.5828	Source: [36]. Calculated as an average of 5 substituted aromatics.
Benzene mixt. with methylbenzene, ethylbenzene, and dimethylbenzene	-	0.9075	Calculated as an average of methylbenzene, ethylbenzene, and dimethylbenzene.
Benzene soluble organics	-	0.9337	Source: [37]

Flowable	CAS No.	Carbon Content (kg C/kg)	Comments
Benzene, methyl benzene, and dimethyl benzene, total	-	0.9088	Calculated as an average of methylbenzene and dimethylbenzene.
Biocides	-	0.3010	Source: [38]. Calculated as an average of 294 biocide ingredients.
Biomass	-	0.5	Assumed. Dry basis.
Biphenyls, polybrominated	-	0.2804	Source: [39]. Calculated as an average of 10 polybrominated biphenyls.
C12-18-Dialkylmethylbenzyl ammonium chlorides	73049-75-9	0.7534	Source: [32]. Assume composition of 60% C14, 30% C16, 5% C18, 5% C12.
C8 Hydrocarbons	93924-38-0	0.8472	Source: [40]. Calculated as an average of 12 C8 hydrocarbons.
Canola oil	120962-03-0	0.7672	Source: [19]. Refined. While canola oil may contain trace amounts of sulfur, iron, copper, and nickel, these compounds are excluded from the carbon content calculations.
Capsicum oleoresins	8023-77-6	0.7038	Source: [42, 43]. Assume 95% capsaicins.
Carbamic acid, salts and esters	-	0.5136	Source: [44, 45]. Calculated as an average of 4 carbamic acid salts and 23 carbamic acid esters.
Carbonodithiocarbonic acids	-	0.3763	Source: [46]. Calculated as an average of 6 carbonodithiocarbonic acids.
Carboxylic acids	-	0.5594	Source: [27]. Calculated as an average of 10 carboxylic acids.
Catalytic cracker distillates C3-11-hydrocarbons	68476-46-0	0.86	Source: [47]. Assume same as distillate fuel oil.
Chlorinated dibenzofurans	136677-10-6	0.3984	Source: [48]. Calculated as an average of 8 chlorinated dibenzofurans.
Chlorinated dibenzo-p-dioxins	136677-09-3	0.4584	Source: [49]. Calculated as an average of 12 chlorinated dibenzo-p-dioxins.
Chlorinated dioxins and furans -- 2,3,7,8 congeners only	-	0.4594	Source: [48, 49]
Chlorinated dioxins and furans -- excluding 2,3,7,8 congeners	-	0.4316	Source: [48, 49]
Chlorinated organic compounds	-	0.2951	Source: [50]. Calculated as an average of 20 COCs.
Chlorinated paraffin	-	0.3433	Source: [51, 52]. Calculated as an average of CP-42, CP-52, and CP-70.
Chlorofluorocarbons	-	0.1227	Source: [53]. Calculated as an average of 15 CFCs.
Citrus extract	94266-47-4	0.8494	Source: [54]. Based on an average of three species: *C. x bergamia*, *C. x myrtifolia*, and *C. limon*.
Clam-trol CT-2	193700-05-9	0.7310	Source: [55]. Carbon content of inert ingredients is an average of inert substances registered with the EPA under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) [56].

Flowable	CAS No.	Carbon Content (kg C/kg)	Comments
Coal	-	0.609	Source: [12, 13]. Weighted average of anthracite (1%), bituminous (55%), lignite (6%), and sub-bituminous (38%) coal by global coal reserves.
Coal, anthracite	-	0.781	Source: [12]. U.S. average.
Coal, bituminous	-	0.7	Source: [12]. U.S. average.
Coal, lignite	-	0.412	Source: [12]. U.S. average.
Coal, sub-bituminous	-	0.503	Source: [12]. U.S. average.
Coalbed methane	-	0.547	Source: [14]. Calculated assuming CH_4 content of 71.9% and CO_2 content of 3.11% at extraction, based on U.S. San Juan coalbed methane production. Carbon content of any NGLs in raw gas is excluded.
Crude oil	-	0.846	Source: [15]. Calculated based on IPCC net calorific value and carbon content.
Distillates, low vapor pressure volatile organic compounds	-	0.6579	Source: [57, 58]. Calculated as an average of 25 compounds.
Esters	-	0.5576	Source: [11]. Calculated as an average of 478 esters.
Ethers, glycol and acetates	-	0.5770	Source: [11]. Calculated as an average of 361 ethers.
Halogenated organics	-	0.3319	Source: [11]. Calculated as an average of 387 halogenated organics.
Hardwood	-	0.4841	Source: [16]. Average of 22 hardwood species. Dry basis.
Heavy alkylate naphtha (petroleum)	64741-65-7	0.8456	Source: [59]. Assume same as kerosene.
Herbicides	-	0.5344	Source: [8]. Assume average of Acetamide, 2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)- and 1,3,5-Triazine-2,4-diamine, 6-chloro-N2-ethyl-N4-(1-methylethyl)-.
Hydrocarbons, c4	87741-01-3	0.8442	Source: [60]. Calculated as an average of 8 C4 hydrocarbons.
Hydrocarbons, C4, ethylene-manuf.-by-product	68476-52-8	0.8559	Source: [61]. Assume composition of C4 crude butadiene.
Hydrocarbons, C8	93924-38-0	0.8472	Source: [40]. Calculated as an average of 12 C8 hydrocarbons.
Hydrocarbons, ethylene-manuf.-by-product distn. residues	68921-67-5	0.8825	Source: [20]. Assume composition of pyrolysis gasoline.
Hydrochlorofluorocarbons	-	0.1915	Source: [53]. Calculated as an average of 38 HCFCs.
Hydrofluorocarbons	-	0.2705	Source: [62]. Calculated as an average of 43 HFCs.
Hydrotreated light distillates (petroleum)	64742-47-8	0.8456	Source: [59]. Assume same as kerosene.

Flowable	CAS No.	Carbon Content (kg C/kg)	Comments
IMCO Lube 106	-	0.7416	Source: [63, 64]. Calculated as an average of glycerol monooleate and 11 mixed long-chain alcohols.
IMCO Lubrikleen	-	0.6608	Source: [65, 66]. Calculated as an average of 26 compounds.
IMCO Nos. 1,2,3,6	-	0.8577	Source: [67, 68, 47]
IMCO Nos. 4,5	-	0.8588	Source: [67, 68, 47]
Kerosene	8008-20-6	0.8456	Source: [59]
Macrotrol 9210	-	0.7184	Source: [69]. Carbon content of inert ingredients is an average of inert substances registered with the EPA under FIFRA [56].
Marl	-	0.04174	Source: [70]
Naphtha	8030-30-6	0.8489	Source: [71]
Natural gas	8006-61-9	0.598	Source: [14]. Calculated assuming CH_4 content of 79.5% and CO_2 content of 0.874% at extraction, based on weighted U.S. average conventional gas production. Carbon content of any NGLs in raw gas is excluded.
Neem oil	8002-65-1	0.7489	Source: [72]
Neptune Blue	39409-45-5	0.01	Source: [73]
N-Nitroso compounds, volatile	-	0.4598	Source: [74]. Calculated as an average of 5 n-nitroso compounds.
Oil sand	-	0.08844	Source: [17, 15]. Calculated assuming 10% bitumen in oil sands and bitumen carbon content calculated based on IPCC net calorific value and carbon content.
Oil shale	-	0.2098	Source: [75]. Assumes mineral component is a mix of calcite and dolomite.
Organochlorine pesticides	-	0.3798	Source: [76]. Calculated as an average of 20 organochlorine pesticides.
Oxygenated compounds	-	0.5272	Source: [77, 11]. Calculated as an average of 125 acids, 478 esters, 152 ketones, and 60 aldehydes.
Particulate matter	-	0.2975	Source: [35]. Average of $PM_{2.5}$ and PM_{10} carbon contents.
Particulate matter, > 10µm	-	0.2725	Source: [35]
Particulate matter, > 2.5µm and ≤ 10µm	-	0.2975	Source: [35]. Average of $PM_{2.5}$ and PM_{10} carbon contents.
Particulate matter, ≤ 10µm	-	0.2725	Source: [35]
Particulate matter, ≤ 2.5µm	-	0.3225	Source: [35]
Peat	-	0.3445	Source: [18, 15]. Average of 14 sites (40.7%) and calculated based on IPCC net calorific value and carbon content (28.2%).
Perfluorocarbons	308069-13-8	0.2073	Source: [79]. Calculated as an average of 9 PFCs.

Flowable	CAS No.	Carbon Content (kg C/kg)	Comments
Pesticides	-	0.4708	Source: [80]. Calculated as an average of 3,223 active ingredients in pesticides.
Pesticides, chlorinated	-	0.3798	Source: [76]. Assume same as organochlorine pesticides.
Pesticides, organic, total	-	0.3577	Source: [76]. Calculated as an average of organochlorine and organophosphate pesticides.
Pesticides, organochlorinated and polychlorinated biphenyls, total	-	0.4194	Source: [76]. Calculated as an average of organochlorine pesticides and polychlorinated biphenyls.
Pesticides, phosphated	-	0.3355	Source: [76]. Calculated as an average of 16 organophospate pesticides.
Petroleum	8002-05-9	0.846	Source: [15]. Assume same as crude oil.
Phenols	-	0.5757	Source: [11]. Calculated as an average of 250 phenols.
Polychlorinated biphenyls	1336-36-3	0.4589	Source: [81]. Calculated as an average of 226 PCBs.
Polycyclic aromatic hydrocarbons	130498-29-2	0.9209	Source: [31]. Calculated as an average of 86 PAHs.
Polycyclic aromatic hydrocarbons - 15-PAH	-	0.9510	Source: [82]
Polycyclic aromatic hydrocarbons - 7-PAH	-	0.9501	Source: [37]
Polycyclic aromatic hydrocarbons, PAH15	-	0.9510	Source: [82]
Polycyclic aromatic hydrocarbons, PAH16	-	0.9510	Source: [82]. Assume same as PAH15.
Polycyclic aromatic hydrocarbons, PAH7	-	0.9501	Source: [37]
Primary forest	-	0.5	Assumed. Dry basis.
Priority pollutants	-	0.4426	Source: [72]. Calculated as an average of 129 compounds.
Priority pollutants, acidic	-	0.5120	Source: [72, 73]. Calculated as an average of 11 compounds.
Priority pollutants, basic or neutral	-	0.6558	Source: [72, 73]. Calculated as an average of 45 compounds.
Quassia extract	68915-32-2	0.1709	Source: [85, 86]
Rosemary oil	8000-25-7	0.8159	Source: [20]
Sesame oil	8008-74-0	0.7663	Source: [21]
Shale gas	-	0.591	Source: [14]. Calculated assuming CH_4 content of 78.8% and CO_2 content of 0.435% at extraction, based on weighted U.S. average shale gas production. Carbon content of any NGLs in raw gas is excluded.
Siloxanes, methyl-, volatile	-	0.3575	Source: [89]. Calculated as an average of 9 volatile methylsiloxanes.

Flowable	CAS No.	Carbon Content (kg C/kg)	Comments
Softwood	-	0.5105	Source: [16]. Average of 21 softwood species. Dry basis.
Soy oil	8001-22-7	0.7420	Source: [90]
Sulfonic acids, C13-17-sec-alkane, sodium salts	85711-69-9	0.5682	Calculated as an average of C13–C17.
Surfactants	-	0.6749	Source: [91, 92, 93, 94, 95]. Calculate as an average of several compounds – see documentation for details.
Tannins and lignen, total	-	0.5258	Source: [8]. Calculated as an average of tannin and lignin.
Tea tree oil	68647-73-4	0.8292	Source: [23]
Thiocarbamic acid, salts and esters	-	0.3592	Source: [11]. Calculated as an average of 30 compounds.
Tight gas	-	0.567	Source: [14]. Calculated assuming CH_4 content of 75.2% and CO_2 content of 1.45% at extraction, based on weighted U.S. average tight gas production. Carbon content of any NGLs in raw gas is excluded.
Total oil and grease, less total petroleum hydrocarbons (TPH)	-	0.7638	Source: [97]. Assume mix of 13 vegetable oils.
Total toxic organics	-	0.5069	Source: [98]. Calculated as an average of 111 compounds.
Trihalomethanes (four), total	-	0.0698	Source: [99]. Calculated as an average of chloroform, bromodichloromethane, dibromochloromethane, and bromoform.
Volatile halogenated hydrocarbons	-	0.1599	Source: [100, 101]. Calculated as an average of CFCs, HCFCs, HFCs, Halons, and very short-lived substances.
Volatile halogenated organics (VHO)	-	0.2290	Source: [102]. Calculated as an average of 48 VHOs.
Volatile organic compounds	-	0.3883	Source: [103]. Calculated as an average of 42 VOCs.
Wood	-	0.5	Assumed. Dry basis.
XC Polymer	9046-08-6	0.3943	Source: [104]. Assume same as xanthan gum.