METHYL SOYATE

(CAS #68919-53-9)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: February 25, 2025[1]

Expiration Date: February 25, 2030

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[1] The report was last updated on February 25, 2025. However, the last complete literature search was conducted on December 12, 2024.

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GreenScreen® Executive Summary for Methyl soyate (CAS #68919-53-9)

Methyl soyate belongs to the fatty acid alkyl ester chemical group. It is an unknown or variable composition, complex reaction products or of biological materials (UVCB) chemical that consists of a mixture of long-chain fatty acid methyl esters. It is used as an alternate fuel (biodiesel), solvent, lubricant, in building composites, paints and coatings, plastics, an emulsifier and wetting agent, and as a pesticide carrier and adjuvant. It is produced by reacting soybean oil and methanol via base-catalyzed transesterification of the oil with alcohol, direct acid-catalyzed esterification of the oil with methanol, or conversion of the oil to fatty acids and then to alkyl esters with acid catalysis.

Methyl soyate was assigned a **GreenScreen Benchmark™ Score of 3** ("Use but Still Opportunity for Improvement"). This score is based on the following hazard score combinations:

- Benchmark 3a
  - Moderate Bioaccumulation – B
- Benchmark 3c
  - Moderate Group II* Human (skin sensitization – SnS*)

Data gaps (DG) exist for endocrine activity – E and respiratory sensitization - SnR. As outlined in GreenScreen® Guidance Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), methyl soyate meets requirements for a GreenScreen Benchmark™ Score of 3 despite the hazard data gaps. In a worst-case scenario, if methyl soyate were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

GreenScreen® Hazard Summary Table for Methyl soyate

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	**M**	**R**	**D**	**E**	**AT**	**ST**		**N**		**SnS**	**SnR**	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
						s	r*	s	r*	*	*								
L	**L**	*L*	*L*	DG	**L**	**L**	**L**	*L*	**L**	*M*	DG	**L**	**L**	**L**	*L*	**vL**	*M*	**L**	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Chemical Assessment for Methyl soyate (CAS #68919-53-9)

Method Version: GreenScreen® Version 1.4
Assessment Type[2]: Certified
Assessor Type: Licensed GreenScreen® Profiler

GreenScreen® Assessment (v.1.4) Prepared By:
Name: John Lee, M.P.H.
Title: Toxicologist
Organization: ToxServices LLC
Date: December 3, 2024; February 18, 2025

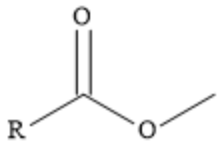
Quality Control Performed By:
Name: Jennifer Rutkiewicz, Ph.D.
Title: Senior Toxicologist
Organization: ToxServices LLC
Date: December 12, 2024; February 25, 2025

Expiration Date: February 25, 2030[3]

Chemical Name: Methyl soyate

CAS Number: 68919-53-9

Chemical Structure(s):



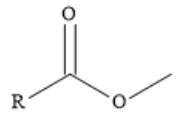
Methyl soyate (CAS #68919-53-9, alt CAS #67784-80-9) has a variable fatty ester composition (TSCA UVCB) in which R groups are generally C16-18 with one to three alkene groups in each chain (CSWG 2000).

Also called:
Fatty acids, soya, Me esters; Soya fatty acids, Me esters (PubChem 2024)

Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
Limited data were identified for methyl soyate, specifically. In addition to alternate CAS #67784-80-9, a supplier SDS has identified CAS #67762-38-3, fatty acids, C16-18 and C18-unsatd., Me esters as an alternate CAS number for this chemical (Stepan 2021). Therefore, data on this CAS number were used to fill data gaps. It is unclear if this chemical is derived specifically from soybean oil, but regardless, fatty acids, C16-18 and C18-unsatd., Me esters is also a UVCB chemical consisting of a mixture of long-chain fatty acid methyl esters with carbon lengths C16, C18 and C18 unsaturated. In addition, data for rape oil, Me ester (CAS #73891-99-3) were used as this substance is identified as a key read across chemical in the ECHA REACH dossier for fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3) and is a similar UVCB ingredient derived from rapeseed oil rather than soybean oil (ECHA CHEM 2024). Individual carbon chain length constituents were also used to fill data gaps when needed. Rape oil, Me ester and other surrogates consisting of a combination of multiple similar constituents are considered strong surrogates. The single constituents are weaker surrogates, but data

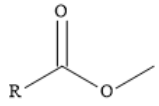
[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), or "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent).
[3] Assessments expire five years from the date of completion starting from January 1, 2019. An assessment expires three years from the date of completion if completed before January 1, 2019 (CPA 2018a).

from multiple surrogates of varying lengths support confidence in the classifications. Although the ECHA REACH dossier included data on additional UVCBs with varying carbon chain lengths, these data were insufficient to fill data gaps or increase confidence; therefore, this assessment relies on data on only the strongest surrogates.



Where R = C15-17 and C17 unsaturated

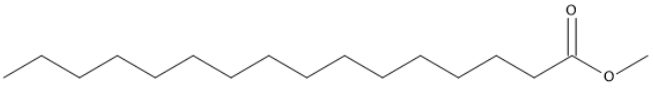
Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3)



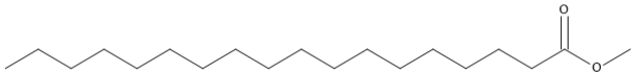
Where R = Fatty acid chains derived from rape oil

Rape oil, Me ester (CAS #73891-99-3)

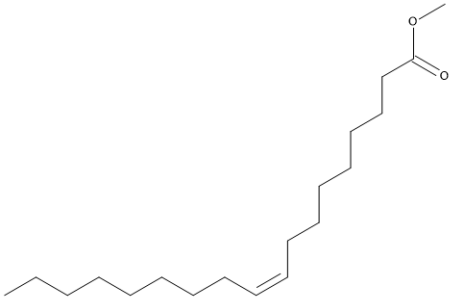
Representative constituents of fatty acids, C16-18 and C18-unsatd., Me Esters are presented below:



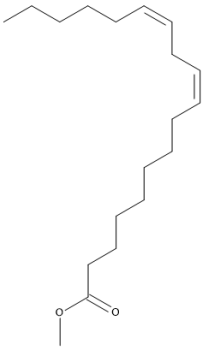
Methyl palmitate (CAS #112-39-0)



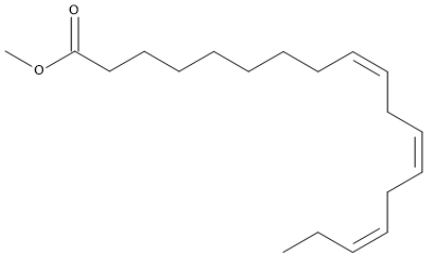
Methyl stearate (CAS #112-61-8)



Methyl oleate (CAS #112-62-9)



Methyl linoleate (CAS #112-63-0)



Methyl linolenate (CAS #301-00-8)

Identify Applications/Functional Uses:
1. Solvent
2. Lubricant
3. Emulsifier

Known Impurities[4]:
Based on the manufacturing process, methanol is a potential residual. The screen is performed on the theoretical pure substance.

GreenScreen® Summary Rating for Methyl soyate[5,6 7,8]: Methyl soyate was assigned a **GreenScreen Benchmark™ Score of 3** ("Use but Still Opportunity for Improvement") (CPA 2018b). This score is based on the following hazard score combinations:

- Benchmark 3a
  - Moderate Bioaccumulation – B
- Benchmark 3c
  - Moderate Group II* Human (skin sensitization – SnS*)

Data gaps (DG) exist for endocrine activity – E and respiratory sensitization - SnR. As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), methyl soyate meets requirements for a GreenScreen Benchmark™ Score of 3 despite the hazard data gaps. In a worst-case scenario, if methyl soyate were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Summary for Methyl soyate

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F
						s	r*	s	r*	*	*								
L	**L**	*L*	*L*	DG	**L**	**L**	**L**	*L*	**L**	*M*	DG	**L**	**L**	**L**	*L*	**vL**	*M*	**L**	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

Environmental Transformation Products
Per GreenScreen® guidance (CPA 2018b), chemicals that degrade rapidly and completely (i.e., meet criteria for a Very Low for persistence) are not likely to form persistent biodegradation intermediates because the degradation intermediates will not persist long enough to be encountered after use or release

[4] Impurities of the chemical will be assessed at the product level instead of in this GreenScreen®.
[5] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.
[6] See Appendix A for a glossary of hazard endpoint acronyms.
[7] For inorganic chemicals only, see GreenScreen® Guidance v1.4 Section 12 (Inorganic Chemical Assessment Procedure).
[8] For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen® Guidance v1.4 Annex 2.

of the parent chemical (i.e., relevant). As methyl soyate is readily biodegradable, it is not expected to have relevant transformation products.

Introduction

Methyl soyate belongs to the fatty acid alkyl ester chemical group. It is used as an alternate fuel (biodiesel), solvent, lubricant, in building composites, paints and coatings, plastics, an emulsifier and wetting agent, and as a pesticide carrier and adjuvant. It is produced by reacting soybean oil and methanol via base-catalyzed transesterification of the oil with alcohol, direct acid-catalyzed esterification of the oil with methanol, or conversion of the oil to fatty acids and then to alkyl esters with acid catalysis.

ToxServices assessed methyl soyate against GreenScreen® Version 1.4 (CPA 2018b) following procedures outlined in ToxServices' SOPs (GreenScreen® Hazard Assessment) (ToxServices 2021).

U.S. EPA Safer Choice Program's Safer Chemical Ingredients List

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2024a). It can be accessed at: http://www2.epa.gov/saferchoice/safer-ingredients. Chemicals on the SCIL have been assessed for compliance with the Safer Choice Standard and Criteria for Safer Chemical Ingredients (U.S. EPA 2024b).

Methyl soyate is listed on SCIL as a Green Half-Circle.

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen Benchmark™ 1 chemicals (CPA 2018b). Pharos (Pharos 2024) is an online list-searching tool that is used to screen chemicals against all of the lists in the List Translator electronically. ToxServices also checks the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b),[9] which are not considered GreenScreen® Specified Lists but are additional information sources, in conjunction with the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for methyl soyate can be found in Appendix C.

- Methyl soyate is an LT-UNK chemical when screened using Pharos, and therefore a full GreenScreen® is required.
- Methyl soyate is not listed on the U.S. DOT list.
- Methyl soyate is on the following list for multiple endpoints. Specified lists for single endpoints are reported in individual hazard endpoints in the hazard assessment section below.
    - German FEA - Substances Hazardous to Waters (Class 1 - Low Hazard to Waters).

Hazard Statement and Occupational Control

No Globally Harmonized System of Classification and Labelling of Chemicals (GHS) hazard statements were identified for methyl soyate, as indicated in Table 1. General personal protective equipment (PPE) recommendations are presented in Table 2, below. No occupational exposure limits (OELs) were identified.

[9] DOT lists are not required lists for GreenScreen® List Translator v1.4. They are reference lists only.

Table 1: GHS H Statements for Methyl soyate (CAS #68919-53-9) (ECHA 2024)	
H Statement	**H Statement Details**
No harmonized GHS H statements are reported by the European Chemicals Agency (ECHA). According to the notifications provided by companies to ECHA in REACH registrations, no hazards have been classified.	

Table 2: Occupational Exposure Limits and Recommended Personal Protective Equipment for Methyl soyate (CAS #68919-53-9)			
Personal Protective Equipment (PPE)	**Reference**	**Occupational Exposure Limits (OEL)**	**Reference**
Gloves and safety glasses/goggles	Stepan 2021	None	N/A

Physicochemical Properties of Methyl soyate

Methyl soyate is a UVCB chemical that is a clear to amber liquid at standard temperature and pressure. It is insoluble in water and may be volatile based on a reported vapor pressure as high as 3.12 mmHg at 20°C. A partition coefficient was not identified.

Table 3: Physical and Chemical Properties of Methyl soyate (CAS #68919-53-9)		
Property	**Value**	**Reference**
Molecular formula	Unspecified (UVCB)	PubChem 2024
SMILES Notation	Unspecified (UVCB)	PubChem 2024
Molecular weight	Unspecified (UVCB)	PubChem 2024
Physical state	Liquid	PubChem 2024
Appearance	Clear, amber to colorless	AGP 2015 Stepan 2014
Melting point	0.1°C (exp.)	Stepan 2014
Boiling point	352°C (exp.)	Stepan 2014
Vapor pressure	3.12 mmHg at 20°C (exp.) 6.8 Pa (0.05 mmHg) at 20°C (exp. For fatty acids, C16-18 and C18-unsatd., Me esters) 3.6 mBar (2.7 mmHg) at 20°C (exp. for fatty acids, C16-18 and C18-unsatd., Me esters)	Stepan 2014 ECHA CHEM, CAS # 68919-53-9, 2024
Water solubility	Insoluble < 0.023 mg/L (exp. for fatty acids, C16-18 and C18-unsatd., Me esters)	Stepan 2014 ECHA CHEM, CAS # 68919-53-9, 2024
Dissociation constant	Not identified	
Density/specific gravity	0.88 g/mL (exp.)	Stepan 2014
Partition coefficient	Log Kow = 8.02 (est.) Log K_{ow} = 7.45 (exp.)	U.S. EPA 2017

Toxicokinetics

Higher molecular weight fatty acid methyl esters are readily hydrolyzed to the corresponding alcohol and acid and then generally oxidized to carbon dioxide and water via breakdown into two-carbon fragments which are used by the body for energy and building blocks for synthesis. During digestion, they are hydrolyzed to the free fatty acids for absorption from the intestine into the blood aided by lipase

enzymes and bile salts. Once formed, the free fatty acid is metabolized by known oxidative processes or reconstituted into glyceride esters and stored in the fat depots of the body (CSWG 2000).

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): *L*
Methyl soyate was assigned a score of Low for carcinogenicity based on negative results in oral and dermal carcinogenicity studies on multiple constituents. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as the studies are lacking in detail.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Oral: Surrogate: Methyl oleate (CAS #112-62-9):* When consumed in feed by mice, methyl oleate did not demonstrate carcinogenic activity during the 300 day exposure period or the following 28 week observation period (equivalent or similar to EU Method B.32, non-GLP). No further details were provided (Klimisch 2, reliable with restrictions).
  - *Dermal: Surrogate: Methyl oleate (CAS #112-62-9):* When applied dermally to the skin of mice, methyl oleate did not demonstrate carcinogenic activity during the 1 year exposure period or the following 1 year observation period (equivalent or similar to EU Method B.32, non-GLP). No further details were provided (Klimisch 2, reliable with restrictions).
  - *Subcutaneous: Surrogate: Methyl stearate (CAS #112-61-8):* When injected subcutaneously in mice, methyl stearate did not demonstrate carcinogenic activity during the 26 week exposure period or the following 18-24 month observation period (non-guideline, non-GLP). No further details were provided (Klimisch 2, reliable with restrictions).
- CSWG 2000
  - *Oral: Surrogate: Methyl oleate (CAS #112-62-9):* When given in the feed, methyl oleate did not demonstrate carcinogenic activity during the 2-year observation period. No further details were provided.
  - *Oral: Surrogate: Methyl linoleate (CAS #112-63-0):* Methyl linoleate was tested for carcinogenicity toward the GI tract in male Wistar rats. No effect as a complete carcinogen was reported and it did not enhance the carcinogenesis of N-methyl-N-nitro-nitrosaguanidine (MNNG) when fed by stomach tube for a maximum of 612 days. No further details were provided.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): L
Methyl soyate was assigned a score of Low for mutagenicity/genotoxicity based on negative results from strong surrogates in bacterial reverse mutation assays and a chromosomal aberration test. GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when negative data are available for both gene mutations and chromosome aberrations, and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data on the target chemical and strong surrogates.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

- ECHA CHEM, CAS #67762-38-3, 2024
    - *In vitro:* *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd., Me esters was negative in a GLP-compliant OECD Guideline 471 bacterial reverse mutation assay in which *Salmonella typhimurium* test strains TA98, TA100, TA102, TA1535, and TA1537 were exposed to the test substance at 0, 62.5, 125, 250, 500, and 1,000 µg/plate with and without metabolic activation in experiment 1 and 0, 312.5, 625, 1,250, 2,500, and 5,000 µg/plate with and without metabolic activation in experiment 2. There was no cytotoxicity. Positive and vehicle controls were valid (Klimisch 1, reliable without restriction).
    - *In vitro:* *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* Rape oil, Me ester was negative in a GLP-compliant OECD Guideline 471 bacterial reverse mutation assay in which *S. typhimurium* test strains TA98, TA100, TA1535, and TA1537 were exposed to the test substance at 5 - 5,000 µg/plate with and without metabolic activation. There was no cytotoxicity. Positive and vehicle controls were valid (Klimisch 2, reliable with restrictions).
    - *In vitro:* *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd., Me esters was negative in a GLP-compliant OECD Guideline 473 chromosome aberration assay in which primary lymphocyte cells were exposed to the test substance at 18.96, 37.93, 75.85, 151.70, 303.41, 606.82, 1,213.64, and 2,427.27 µg/mL with and without metabolic activation in experiment 1 and 75.85, 151.70, 303.41, 606.82, 1,213.64, and 2,427.27 µg/mL with and without metabolic activation in experiment 2. There was no cytotoxicity. Positive and vehicle controls were valid (Klimisch 1, reliable without restriction).
- NTP 2024
    - *In vitro:* Methyl soyate was negative in a bacterial reverse mutation assay in which *S. typhimurium* test strains TA97, TA98, TA100, and TA1535, were exposed to the test substance at 0, 333, 1,000, 3,333, and 10,000 µg/plate with and without metabolic activation. No further details were provided.
    - *In vivo:* Methyl soyate was negative in a micronucleus assay in which male B6C3F1 mice (5/dose) were administered the test substance at a dose of 500, 1,000, and 2,000 mg/kg via gavage. No further details were provided.

Reproductive Toxicity (R) Score (H, M, or L): *L*

Methyl soyate was assigned a score of Low for reproductive toxicity based on a lack of reproductive effects in a screening study on a strong surrogate. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on a screening study on a strong surrogate.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
    - *Oral:* *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* In a GLP-compliant combined repeated dose and reproduction/developmental toxicity screening study, conducted in accordance with OECD Guideline 422, Sprague-Dawley rats (10/sex/dose) were treated with 0, 100, 300, or 1,000 mg/kg/day fatty acids, C18-18 and C18-unsatd., Me esters (99.35% purity) once daily via oral gavage. Males were treated once daily for four weeks and females were treated two weeks before pairing, during mating and

gestation, until 4 days post-partum. No effects on reproductive performance were observed. No clinical signs of toxicity or mortality were reported in pups. No changes in pup body weight or pup weight gain were measured compared to controls. Study investigators identified a reproductive NOAEL of 1,000 mg/kg/day based on a lack of treatment-related effects (Klimisch 2, reliable with restrictions).

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): *L*
Methyl soyate was assigned a score of Low for developmental toxicity based on a lack of developmental effects in a screening study on a strong surrogate. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on a screening study on a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Oral: Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* In the previously described GLP-compliant combined repeated dose and reproduction/developmental toxicity screening study, conducted in accordance with OECD Guideline 422, Sprague-Dawley rats (10/sex/dose) were treated with 0, 100, 300, or 1,000 mg/kg/day fatty acids, C18-18 and C18-unsatd., Me esters (99.35% purity) once daily via oral gavage. Males were treated once daily for four weeks and females were treated two weeks before pairing, during mating and gestation, until 4 days post-partum. No abnormalities were found in the pups. No clinical signs of toxicity or mortality were reported in pups. No changes in pup body weight or pup weight gain were measured compared to controls, and there were no treatment-related effects on gross pathology or histopathology. Study investigators identified a developmental NOAEL of 1,000 mg/kg/day based on a lack of treatment-related effects (Klimisch 2, reliable with restrictions).

Endocrine Activity (E) Score (H, M, or L): DG
Methyl soyate was assigned a score of Data Gap for endocrine activity based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- No data were identified.

Group II and II* Human Health Effects (Group II and II* Human)
Note: Group II and Group II* endpoints are distinguished in the v 1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. See GreenScreen® Guidance v1.4, Annex 2 for more details.

Acute Mammalian Toxicity (AT) (Group II) Score (vH, H, M, or L): L
Methyl soyate was assigned a score of Low for acute toxicity based on oral LD_{50} values > 5,000 mg/kg. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when oral LD_{50} values are > 2,000 mg/kg (CPA 2018b). The confidence in the score is high as it is based on reliable data from studies on the target chemical and a strong surrogate.

- Authoritative and Screening Lists

  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Oral:* *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* LD_{50} (male and female Sprague-Dawley rat) > 5,000 mg/kg (equivalent or similar to OECD Guideline 401, GLP compliant) (Klimisch 1, reliable without restriction).
- CSWG 2000
  - *Oral:* LD_{50} (species not identified) >17.4 g/kg

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-single) (Group II) Score (vH, H, M, or L): L

Methyl soyate was assigned a score of Low for systemic toxicity (single dose) based on a NOAEL of 5,000 mg/kg/day from an acute oral study on a strong surrogate. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (single dose) when there is no evidence or systemic toxicity below the oral guidance value of 2,000 mg/kg and no GHS classification are available (CPA 2018b). The confidence in the score is high as it is based on reliable data from a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Oral:* *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C18-18 and C18-unsatd., Me esters was administered to male and female Sprague-Dawley rats in an acute oral toxicity study (equivalent or similar to OECD Guideline 401, GLP-compliant). The unchanged test substance was administered by gavage at 10 mL/kg (reported equivalent to 5,000 mg/kg). No mortality was observed. From 10 minutes to 3 hours after administration, decreased body movement was noticed in all animals. There were no clinical signs from 3 hours to day 14. No effect on body weight was observed at the end of the observation period. No macroscopic findings were recorded at necropsy (Klimisch 1, reliable without restriction). *ToxServices assigned a NOAEL of 5,000 mg/kg/day for systemic toxicity.*

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-repeat) (Group II*) Score (H, M, or L): L

Methyl soyate was assigned a score of Low for systemic toxicity (repeated dose) based on an oral NOAEL of 1,000 mg/kg/day in a combined repeated dose and reproduction/developmental toxicity screening study on a strong surrogate. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when the oral LOAEL is > 100 mg/kg/day in a 90-day study, adjusted to 300 mg/kg/day for a 28-day study (CPA 2018b). The confidence in the score is high as it is based on reliable data from a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Oral:* *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* In the previously described GLP-compliant combined repeated dose and reproduction/developmental toxicity screening study, conducted in accordance with OECD Guideline 422, Sprague-Dawley rats (10/sex/dose) were treated with 0, 100, 300, or 1,000 mg/kg/day fatty acids, C18-18 and C18-unsatd., Me esters (99.35% purity) once daily via

oral gavage. Males were treated once daily for four weeks and females were treated two weeks before pairing, during mating and gestation, until 4 days post-partum. Two animals died prematurely; however, the deaths were not related to treatment. No treatment-related changes in body weight, weight gain, or food consumption were reported. No abnormalities were observed during ophthalmological or histopathological examination. Increased percent red cell distribution was noted in males at 100 mg/kg/day, but was not reported in any other dose group or associated with any other hematological changes and therefore considered incidental. Increased potassium was reported in males at 100 mg/kg/day, but was not reported in any other dose group or associated with any other hematological changes and therefore considered incidental. Study investigators identified a systemic NOAEL of 1,000 mg/kg/day based on a lack of treatment-related effects (Klimisch 1, reliable without restriction). *ToxServices adjusted the guidance value to reflect that this was a four week study instead of a 90-day study; therefore, the NOAEL is compared to a tripled guidance value of 300 mg/kg/day.*

Neurotoxicity (single dose, N-single) (Group II) Score (vH, H, M, or L): *L*
Methyl soyate was assigned a score of Low for neurotoxicity (single dose) based on a lack of specific signs of neurotoxicity at an acute oral dose of 5,000 mg/kg/day. GreenScreen criteria classify chemicals as a Low hazard for neurotoxicity (single dose) when there is no evidence of neurotoxicity below the oral guidance value of 2,000 mg/kg/day and no GHS classifications are available (CPA 2018b). The confidence is low because acute studies do not include specific evaluations of neurotoxicity.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Oral: Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C18-18 and C18-unsatd., Me esters was administered to male and female Sprague-Dawley rats in an acute oral toxicity study (equivalent or similar to OECD Guideline 401, GLP-compliant). The test substance was administered by gavage unchanged at 10 mL/kg (reported equivalent to 5,000 mg/kg). No mortality was observed. From 10 minutes to 3 hours after administration, decreased body movement was noticed in all animals. There were no clinical signs from 3 hours to day 14. No macroscopic findings were recorded at necropsy (Klimisch 1, reliable without restriction). *Although decreased body weight is potentially indicative of neurotoxicity, ToxServices did not consider this effect suitable for classification for neurotoxicity or transient narcotic effects as it is likely a nonspecific effect due to administration of a large bolus dose, and no additional signs of neurotoxicity were noted..*

Neurotoxicity (repeated dose, N-repeated) (Group II*) Score (H, M, or L): L
Methyl soyate was assigned a score of Low for neurotoxicity (repeated dose) based on an oral NOAEL of 1,000 mg/kg/day in a combined repeated dose and reproduction/developmental toxicity screening study on a strong surrogate that included a functional battery. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (repeated dose) when the oral LOAEL is > 100 mg/kg/day in a 90-day study, adjusted to 300 mg/kg/day for a 28-day study (CPA 2018b). The confidence in the score is high as it is based on reliable data from a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024

- *Oral: <u>Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):</u>* In a GLP-compliant combined repeated dose and reproduction/developmental toxicity screening study, conducted in accordance with OECD Guideline 422, Sprague-Dawley rats (10/sex/dose) were treated with 0, 100, 300, or 1,000 mg/kg/day fatty acids, C18-18 and C18-unsatd., Me esters (99.35% purity) once daily via oral gavage. Males were treated once daily for four weeks and females were treated two weeks before pairing, during mating and gestation, until 4 days post-partum. During week 4 for males and during lactation for females, a functional assessment, including, grip strength, pain perception, landing foot splay, and motor activity, was conducted on 5 animals/sex/dose. No effects were reported and a neurotoxicity NOAEL of 1,000 mg/kg/day can be established for this study (Klimisch 2, reliable with restrictions). *ToxServices adjusted the guidance value to reflect that this was a four week study instead of a 90-day study; therefore, the NOAEL is compared to a tripled guidance value of 300 mg/kg/day.*

Skin Sensitization (SnS) (Group II*) Score (H, M, or L): *M*

Methyl soyate was assigned a score of Moderate for skin sensitization based on positive results in a mouse LLNA leading to a Category 1B classification. GreenScreen® criteria classify chemicals as a Moderate hazard for skin sensitization when they are GHS Category 1B (CPA 2018b). The confidence in the score is low as the study details in the positive LLNA are lacking and insufficient to conclusively subclassify, and results conflict with a negative guinea pig maximization test.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *<u>Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):</u>* Fatty acids, C16-18 and C18-unsatd., me esters was not dermally sensitizing in a GLP-compliant, OECD Guideline 406 guinea pig maximization test. Male and female Hartley guinea pigs (10/sex treated, 5/sex control) were intradermally and epicutaneously induced with 75% and 100% test substance in corn oil, respectively, and epicutaneously challenged with undiluted test substance under occlusive conditions. At 24 and 48 hours after challenge, 0/20 animals displayed positive sensitization reactions (Klimisch 1, reliable without restriction).
- U.S. EPA 2013a
  - In a mouse local lymph node assay (LLNA) female CBA/JHsd mice (5/group) were administered 0% (vehicle – propylene glycol) or 100% soybean oil, me esters for 3 consecutive days. An increase in cell proliferation and a stimulation index (SI) greater than 3 was reported with 100% test substance; however, an EC3 value could not be calculated because the summary did not report results for different test concentrations.
- Based on the weight of evidence, a score of Moderate was assigned. Though the results of the LLNA test are positive for sensitization, the study details are not sufficient to subclassify methyl soyate as a Category 1A or 1B skin sensitizer. The substance was only tested at 100% and no EC3 value could be calculated. Additionally, the results from a guinea pig maximization test do not support the positive results from the LLNA. As there is no evidence in the literature that fatty acid alkyl esters are have a high potency or high frequency of occurrence of skin sensitization, the dose reported to have an EC3 in the LLNA was much greater than 20%, and the guinea pig maximization test was negative, ToxServices did not consider the data sufficient to assign a Category 1A classification, and therefore classified methyl soyate to Category 1B.

Respiratory Sensitization (SnR) (Group II*) Score (H, M, or L): DG
Methyl soyate was assigned a score of Data Gap for respiratory sensitization based on a lack of data for this endpoint.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2024
  - *Surrogate: Methyl oleate (CAS #112-62-9):* Methyl oleate does not contain any structural alerts for respiratory sensitization (Appendix D),
- No data were identified for the target compound for this endpoint. Therefore, ToxServices attempted to evaluate the respiratory sensitization potential of Methyl soyate according to ECHA's guideline (ECHA 2017), which states that the mechanisms leading to respiratory sensitization are essentially similar to those leading to skin sensitization (ECHA 2017). ECHA recommended that if a chemical is not a dermal sensitizer based on high quality data, it is unlikely to be a respiratory sensitizer. ECHA also noted that this rationale does not cover respiratory hypersensitivity caused by non-immunological mechanisms, for which human experience is the main evidence of activity (ECHA 2017). Methyl soyate may be a skin sensitizer based on a positive LLNA. According to the ECHA guidance, the positive skin sensitization results in animals and lack of structural alerts and evidence of respiratory sensitization indicate that there is insufficient positive data for the chemical to be classified as a respiratory sensitizer. However, the guidance requires negative skin sensitization data in order to conclude that the chemical is not a respiratory sensitizer. GreenScreen® criteria require negative data in order to assign a Low (i.e., a lack of alerts is not sufficient). Due to a positive LLNA for skin sensitization and uncertainty regarding whether the mechanisms of sensitization could correspond to respiratory sensitization, and a lack of structural alerts for skin sensitization based on a representative constituent, methyl oleate), a Data Gap was assigned.

Skin Irritation/Corrosivity (IrS) (Group II) Score (vH, H, M, or L): L
Methyl soyate was assigned a score of Low for skin irritation/corrosivity based on negative results in rabbit studies with strong surrogates. GreenScreen® criteria classify chemicals as a Low hazard for skin irritation/corrosivity when negative data and no GHS classification are available (CPA 2018b). The confidence in the score is high as it is based on reliable data from studies on strong surrogates.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd., me esters was slightly irritating to the skin (not sufficient for classification) in a GLP-compliant OECD Guideline 404 acute dermal irritation assay. New Zealand white rabbits (n=6) were administered unchanged test substance to clipped skin for 4 hours under semi-occlusive conditions. Slight erythema was observed in all animals after one hour exposure and disappeared by 48 hours. No edema was reported. The mean (24, 48 and 72 hour) erythema and edema scores for all animals were 0-0.33/4 and 0/4, respectively. A score of 0.33 is below the threshold of 1.5 for classification (Klimisch 1, reliable without restriction).
  - *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* Rape oil, Me ester was slightly irritating to the skin (not sufficient for classification) in a non-GLP-compliant OECD Guideline 404 acute dermal irritation assay. New Zealand white rabbits (n=3) were administered

unchanged test substance to shaved skin for 3 hours under occlusive conditions. Slight erythema was observed in all animals after one hour exposure and was reversible by 24 hours. No edema was reported. The mean (24, 48 and 72 hour) erythema and edema scores for all animals were 0/4 and 0/4, respectively (Klimisch 2, reliable with restrictions).

Eye Irritation/Corrosivity (IrE) (Group II) Score (vH, H, M, or L): L

Methyl soyate was assigned a score of Low for eye irritation/corrosivity based on negative results in rabbit studies with strong surrogates. GreenScreen® criteria classify chemicals as a Low hazard for eye irritation/corrosivity when negative data and no GHS classification are available (CPA 2018b). The confidence in the score is high as it is based on reliable data from studies on strong surrogates.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- Source
  - *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd., me esters was slightly irritating to the eyes (not sufficient for classification) in a GLP-compliant OECD Guideline 405 acute ocular irritation assay. One eye of New Zealand white rabbits (n=6) was instilled with 0.1 mL unchanged test substance and left unrinsed. Conjunctivae effects were observed 1 hour after exposure, with slight chemosis and slight conjunctivae in two and four animals, respectively. Two animals presented conjunctivae with diffuse, crimson color and individual vessels not easily discernible. These effects were fully reversible within 1 day. The mean (24, 48 and 72 hour) chemosis, conjunctiva, iris, and cornea opacity scores were, 0/4, 0.16/3 (maximum of 0.33 for any individual animal), 0/2, and 0/4, respectively. These scores are below the thresholds of 1 and/or 2 for classification (Klimisch 1, reliable without restriction).
  - *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* Rape oil, Me ester was not irritating to the eyes in a non-GLP-compliant OECD Guideline 405 acute ocular irritation assay. One eye of New Zealand white rabbits (n=3) was instilled with 0.1 mL unchanged test substance. Slight irritation was observed one hour after treatment that was reversible in a few hours. Slight erythema was observed in all animals after one hour exposure and was reversible by 24 hours. The mean (24, 48 and 72 hour) chemosis, conjunctiva, iris, and cornea opacity scores were 0/4, 0/3, 0/2, and 0/4, respectively (Klimisch 2, reliable with restrictions).

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): L

Methyl soyate was assigned a score of Low for acute aquatic toxicity based on L/EC_{50} values > 1,000 mg/L for all trophic levels for methyl soyate and rape oil, Me ester. As all values are well above the water solubility of methyl soyate, no effects are expected at saturation. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic toxicity when acute aquatic toxicity values are greater than 100 mg/L (CPA 2018b). The confidence in the score is high as it is based on reliable data from studies on the target chemical and a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- CSWG 2000
  - 96 hour LC_{50} (*Lepomis macrochirus*, bluegill) > 1,000 mg/L
- ECHA CHEM, CAS #67762-38-3, 2024

- *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* 48 hour EC_{50} (mortality) (*Danio rerio*, zebrafish) = >100,000 mg/L water accommodated fraction (WAF) (equivalent or similar to OECD Guideline 203, non-GLP) (Klimisch 2, reliable with restrictions).
- *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* 48 hour EC_{50} (mobility) (*Daphnia magna*, water flea) = 2,504 mg/L (WAF) (OECD Guideline 202, non-GLP) (Klimisch 2, reliable with restrictions).
- *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* 72 hour EC_{50} (growth) (*Pseudokirchneriella subcapitata*, green algae) = 73,729 mg/L (WAF) (equivalent or similar to OECD Guideline 201, non-GLP) (Klimisch 2, reliable with restrictions).

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): *L*

Methyl soyate was assigned a score of Low for chronic aquatic toxicity based on estimated chronic aquatic toxicity values > 10 for all trophic levels. GreenScreen® criteria classify chemicals as a Low hazard for chronic aquatic toxicity when chronic aquatic toxicity values are > 10 mg/L (CPA 2018b). The confidence in the score is low as it is based on acute-to-chronic ratios.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2022
  - Methyl soyate belongs to the Esters and Neutral Organics ECOSAR chemical classes. The most conservative predicted chronic values (ChVs) are 0.00018 mg/L in fish, 0.0050 mg/L in daphnia, and 0.0011 mg/L in green algae (Appendix E). ECOSAR reports an experimental log K_{ow} of 7.45 (source not cited), which is below the max log K_{ow} of 8 for the validity range of the model. In addition, these values are less than the predicted water solubility of 0.012 mg/L. Therefore, because the effects occurred within the range of the predicted water solubility and within the range for acceptable log K_{ow}, modeling predicts very high chronic aquatic toxicity (Appendix E).
- U.S. EPA 2013b
  - In the absence of measured data or reliable modeling, an acute-to-chronic ratio may be applied. Methyl soyate and its surrogates belong to the Esters and Neutral Organics ECOSAR chemical classes. For the both the Esters Neutral Organics classes, the acute-to-chronic ratios are 10 for fish, 10 for daphnid, and 4 for green algae. Dividing the most conservative measured L/EC_{50} values by the ratios results in chronic aquatic toxicity values of (1,000 / 10) = 100 mg/L for fish, (2,504 / 10) = 250.4 mg/L for daphnid, and (73,729 / 4) = 18,432.25 mg/L for green algae.
- U.S. EPA 2015
  - The U.S. EPA concluded that ecotoxicology is not a concern for methyl soyate.
- No measured chronic aquatic toxicity data were identified. However, the acute aquatic toxicity values are high (i.e., L/EC_{50}s >1,000 mg/L) in all three trophic levels for the surrogate rape oil, Me ester. Although modeling predicts ChVs corresponding to a Very High, ToxServices notes that this conflicts with acute aquatic toxicity data, which generally corresponds with chronic aquatic toxicity, and that based on experimental water solubility values reported in REACH dossiers for surrogates (< 0.023 mg/L for fatty acids, C16-18 and C18-unsatd., Me esters and 0.0003 mg/L for methyl stearate), the water solubility may be much lower than the value estimated by ECOSAR. Therefore, ToxServices also calculated acute to chronic ratios for all three trophic levels, and all of these values, which are extrapolated from experimental acute data (described above), exceed the guidance value of 10 mg/L. Furthermore, the U.S. EPA also concluded that ecotoxicology is not a concern

for methyl soyate. Therefore, methyl soyate is not likely to be classified as a chronic aquatic hazard based on the calculated ChVs and because the low water solubility indicates no effects at saturation.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): vL

Methyl soyate was assigned a score of Low for persistence based on a surrogate meeting the 10-day window in ready biodegradability tests. GreenScreen® criteria classify chemicals as a Very Low hazard for persistence when the chemical meets the 10-day window for chemicals partitioning primarily to soil (CPA 2018b). Confidence in the score is high because it was based on reliable experimental data from studies on strong surrogates.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd, Me esters was readily biodegradable and met the 10-day window in a GLP-compliant OECD Guideline 301 B CO_2 Evolution test. In this assay, 25.7 mg/L test substance was exposed to aerobic, non-adapted secondary effluent from a biologic treatment plant for 29 days. The test substance degraded 65% in the 10-day window and 75% within 29 days (Klimisch 2, reliable with restrictions).
  - *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* Rape oil, Me ester was readily biodegradable in a non-GLP-compliant OECD Guideline 301 B CO_2 Evolution test. In this assay, 20 mg/L test substance was exposed to aerobic, domestic, non-adapted sewage for 28 days. The test substance degraded 62.6% in the 10-day window and 87.4% within 28 days (Klimisch 2, reliable with restrictions).
  - *Surrogate: Rape oil, Me ester (CAS #73891-99-3):* Rape oil, Me ester was readily biodegradable in a non-GLP-compliant EU Method C.4-C CO_2 Evolution test. In this assay, 10 mg/L test substance was exposed to aerobic, predominately domestic, non-adapted sewage for 28 days. The test substance degraded 66.32-69.01% in 7 days, 77.83-80.72% in 14 days and 85.54-88.49% within 28 days (Klimisch 2, reliable with restrictions).
- U.S. EPA 2017
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that methyl soyate is expected to be readily biodegradable. Fugacity modeling (EQC Default method) predicts 67.4% will partition to sediment with a half-life of 135 days, 28.7% will partition to soil with a half-life of 30 days, and 3.9% will partition to water with a half-life of 15 days (Appendix F).
- Based on the weight of evidence, a score of Very Low was assigned. EPI Suite™ predicts methyl soyate to mainly partition to sediment and soil, experimental data from a reliable study demonstrate that butyl acetate is readily biodegradable, and this result is supported by modeling.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *M*

Methyl soyate was assigned a score of Moderate for bioaccumulation based on a modeled bioaccumulation (BAF) of 500.4. GreenScreen® criteria classify chemicals as a Moderate hazard for bioaccumulation when the BCF/BAF is > 500 and $\leq$ 1,000 (CPA 2018b). The confidence in the score is low as it is based on modeled data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.

  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd, Me esters has a measured BCF of 3 in an OECD Guideline 305 A assay in *Mytilus edulis* (blue mussel) (Klimisch 2, reliable with restrictions).
- U.S. EPA 2017
  - BCFBAF predicts a BAF of 500.6 using the regression based model based on a measured log K_{ow} of 7.45, using the Arnot-Gobas model for the upper trophic level, taking metabolism into consideration (Appendix F).
- Based on a weight of evidence, a conservative score of Moderate was assigned. Although an experimental BCF of 3 is available in the mussel, GHS criteria prioritize fish bioaccumulation data. Furthermore, based on the relatively high experimental log K_{ow} of 7.45 reported in the experimental PhysProp database, accumulation via food is likely to play a role in bioaccumulation, and therefore, the BAF may be more relevant. The modeled BAF of 500.4 corresponds to a Moderate.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): L
Methyl soyate was assigned a score of Low for reactivity based on the results of an auto-ignition test and NFPA/HMIS ratings of 0 for reactivity. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when GHS reactivity classifications are not needed (CPA 2018b). The confidence in the score is high as it is based on measured data from a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd, Me esters has an auto-ignition temperature of 261°C +/- 5°C based on a GLP compliant EU Method A.15 test (Klimisch 1, reliable without restriction).
- AGP 2015
  - The SDS lists a NFPA/HMIS reactivity score of 0.
- Stepan 2021
  - The SDS lists a NFPA/HMIS reactivity score of 0.

Flammability (F) Score (vH, H, M, or L): L
Methyl soyate was assigned a score of Low for flammability based on a flash point of 173°C, which exceeds the classification cutoff of 93°C, in a closed cup test on a strong surrogate. GreenScreen® criteria classify chemicals as a Low hazard for flammability when GHS classification is not warranted (CPA 2018b). The confidence in the score is high as it is based on measured data from a strong surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA CHEM, CAS #67762-38-3, 2024
  - *Surrogate: Fatty acids, C16-18 and C18-unsatd., Me esters (CAS #67762-38-3):* Fatty acids, C16-18 and C18-unsatd, Me esters has a flash point of 173°C in a closed cup test (EU Method A.9, GLP-compliant) (Klimisch 1, reliable without restriction).
- AGP 2015

    - The SDS lists a NFPA/HMIS flammability score of 1.
- Stepan 2021
    - The SDS lists a NFPA/HMIS flammability score of 1.

Use of New Approach Methodologies (NAMs)[10] in the Assessment, Including Uncertainty Analyses of Input and Output

New Approach Methodologies (NAMs) used in this GreenScreen® include *in vitro* testing for mutagenicity and *in silico* modeling for persistence and bioaccumulation. NAMs are non-animal alternative that can be used alone or in combination to provide information for safety assessment (Madden et al. 2020). At present, there is not a uniformly accepted framework on how to report and apply individual NAMs (U.S. EPA 2020, OECD 2020). The expanded application of NAMs greatly amplifies the need to communicate uncertainties associated with their use. As defined by EFSA (2018), uncertainty is "a general term referring to all types of limitations in available knowledge that affect the range and probability of possible answers to an assessment question." The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties (OECD 2020):

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

As shown in Table 4, Type I (input data) uncertainties in methyl soyate's NAMs dataset include lack of experimental data or validated test methods for respiratory sensitization. Methyl soyate's Type II (extrapolation output) uncertainties include limitations of *in vitro* genotoxicity assays in assessing only a few processes in genotoxicity and not completely mimicking *in vivo* metabolism. Some of methyl soyate's type II uncertainties were alleviated by the use of *in vitro* test batteries and/or in combination of *in vivo* data.

Table 4: Summary of NAMs Used in the GreenScreen® Assessment, Including Uncertainty Analyses

Uncertainty Analyses (OECD 2020)	
Type I Uncertainty: Data/Model Input	**Respiratory sensitization**: No experimental data are available and there are no validated test methods. Very limited human evidence on aluminum compounds is confounded by co-exposure with other chemicals under occupational scenarios.
Type II Uncertainty: Extrapolation Output	**Genotoxicity:** The bacterial reverse mutation assay (as defined in OECD Guideline 471) only tests point-mutation inducing activity in non-mammalian cells, and the exogenous metabolic activation system does not entirely mimic *in vivo* conditions[11]. The *in vitro* chromosome aberration assay (OECD Guideline 473) does not measure aneuploidy and it only measures structural chromosomal aberrations. The exogenous metabolic activation system does not entirely mirror *in vivo* metabolism[12]. **Respiratory sensitization**: The OECD Toolbox only identifies structural alerts and does not define applicability domains.

[10] NAMs refers to any non-animal technology, methodology, approach, or combination thereof that inform chemical hazard and risk assessments. NAMs include *in silico*/computational tools, *in vitro* biological profiling (e.g., cell cultures, 2,3-D organotypic culture systems, genomics/transcriptomics, organs on a chip), and frameworks (i.e., adverse outcome pathways (AOPs), defined approaches (DA), integrated approaches to testing and assessment (IATA).
[11] https://www.oecd-ilibrary.org/docserver/9789264071247-en.pdf?expires=1614097593&id=id&accname=guest&checksum=89925F80B9F4BD2FFC6E90F94A0EE427
[12] https://www.oecd-ilibrary.org/docserver/9789264264649-en.pdf?expires=1614098015&id=id&accname=guest&checksum=6A4F9CE52EA974F5A74793DD54D54352

	Additionally, the ECHA guidance (2017), on which the use of OECD Toolbox structural alerts is based, does not evaluate non-immunologic mechanisms for respiratory sensitization.	
Endpoint	**NAMs Data Available and Evaluated? (Y/N)**	**Types of NAMs Data (*in silico* modeling/*in vitro* biological profiling/frameworks)**
Carcinogenicity	N	
Mutagenicity	Y	*In vitro* data: Bacterial reverse mutation assay/ *in vitro* chromosome aberration assay
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	N	
Acute mammalian toxicity	N	
Single exposure systemic toxicity	N	
Repeated exposure systemic toxicity	N	
Single exposure neurotoxicity	N	
Repeated exposure neurotoxicity	N	
Skin sensitization	N	
Respiratory sensitization	Y	*In silico* modeling: OECD Toolbox structural alerts
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	
Chronic aquatic toxicity	Y	*In silico* modeling: ECOSAR
Persistence	Y	*In silico* modeling: EPI Suite™ Non-animal testing: OECD 301 B and EU Method C.4-C Biodegradation tests
Bioaccumulation	Y	*In silico* modeling: EPI Suite™

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APPENDIX A: Hazard Classification Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

® Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

® Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

® Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for Methyl soyate (CAS #68919-53-9)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	**Chemical Name**	**CAS#**	**C**	**M**	**R**	**D**	**E**	**AT**	**STs**	**STr**	**Ns**	**Nr**	**SNS***	**SNR***	**IrS**	**IrE**	**AA**	**CA**	**P**	**B**	**Rx**	**F**
No	**Methyl soyate**	**68919-53-9**	*L*	**L**	*L*	*L*	DG	**L**	**L**	**L**	DG	**L**	*M*	DG	**L**	**L**	**L**	*L*	**vL**	*M*	**L**	**L**

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	No	No		
2	No	No	No	No	No	No	No
3	Yes	No	Yes	No			
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Methyl soyate	3

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

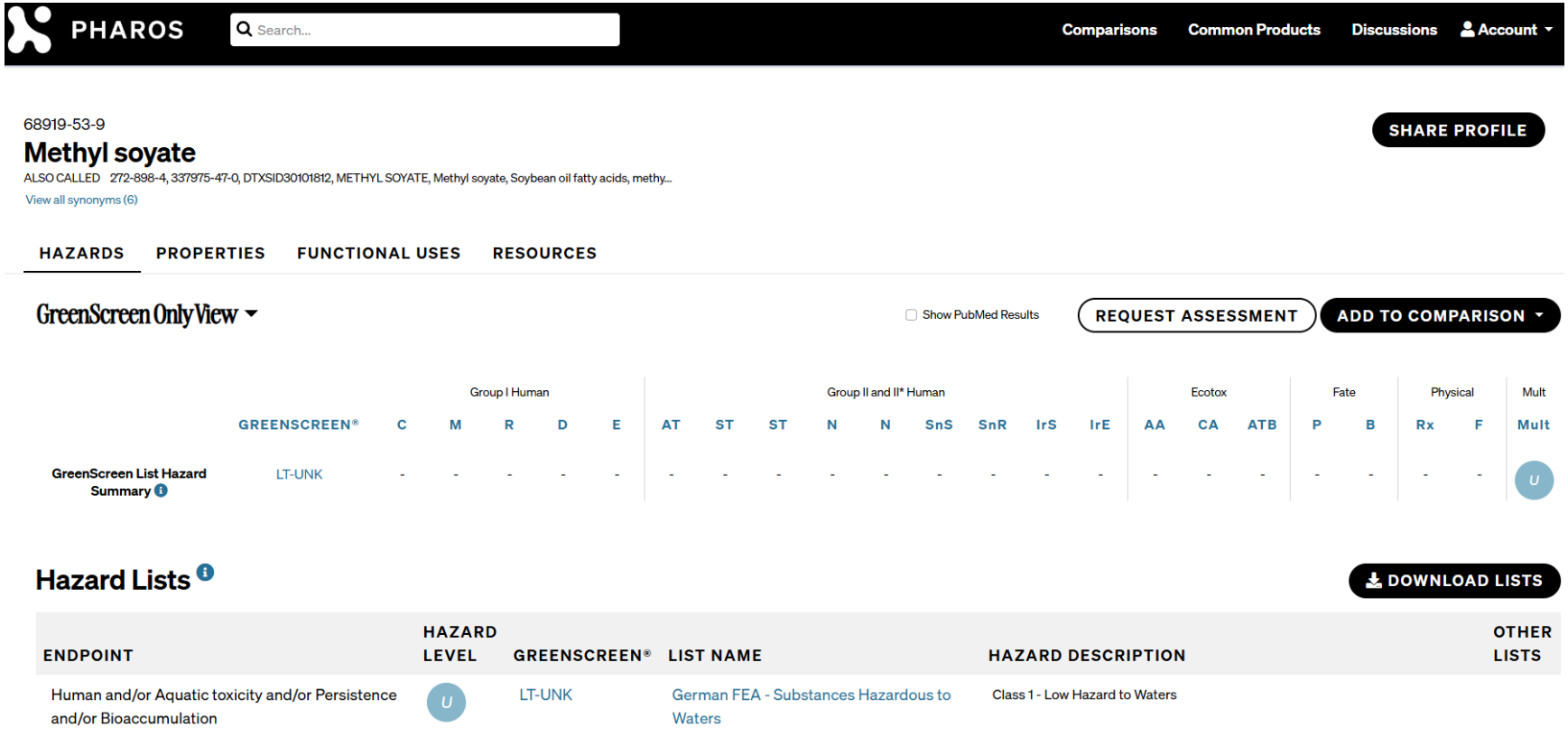
Chemical Name	Final GreenScreen® Benchmark Score
Methyl soyate	3

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												
2												
3	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes		3
4												

APPENDIX C: Pharos Output for Methyl soyate (CAS #68919-53-9)



Restricted Substance Lists (3)

- EC - CEPA DSL: DSL-all
- Food Contact Chemicals Database (FCCdb): Food Contact Chemicals Database Version 5.0
- TSCA Chemical Substance Inventory (Active-Inactive): TSCA Commercially Active

Positive Lists (2)

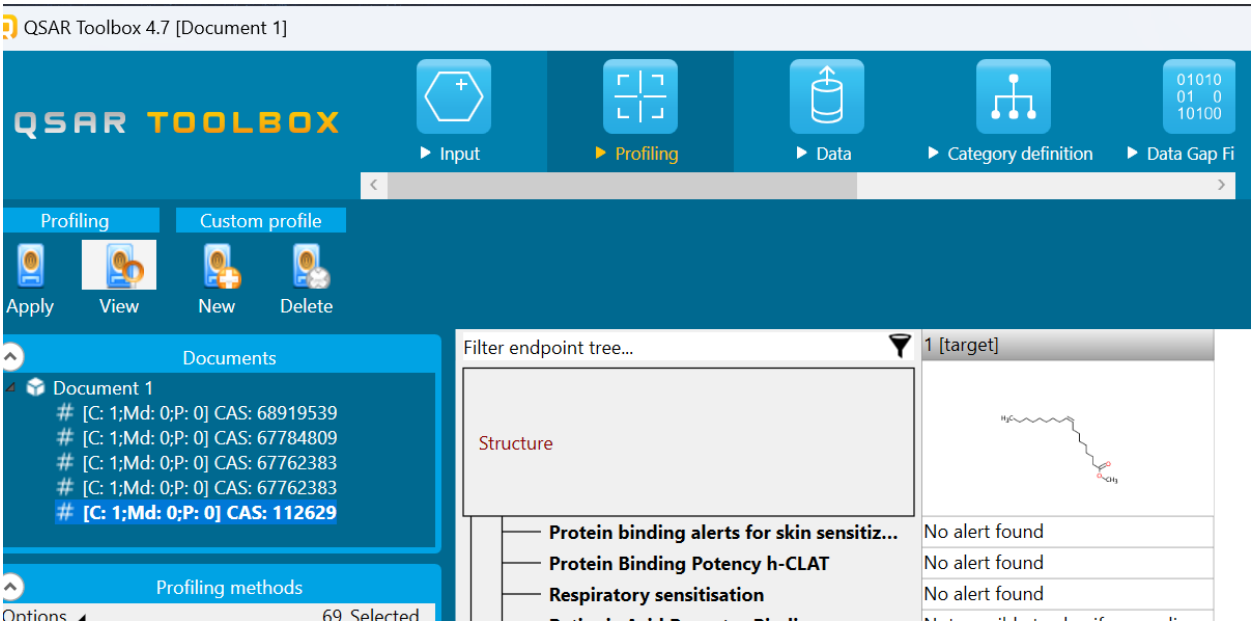
- Inventory of Existing Cosmetic Ingredients in China (IECIC 2021): Cosmetic Ingredients
- US EPA - DfE Safer Chemicals Ingredients list (SCIL): Solvents - Green Half-Circle (Expected Low Concern)

Discussions

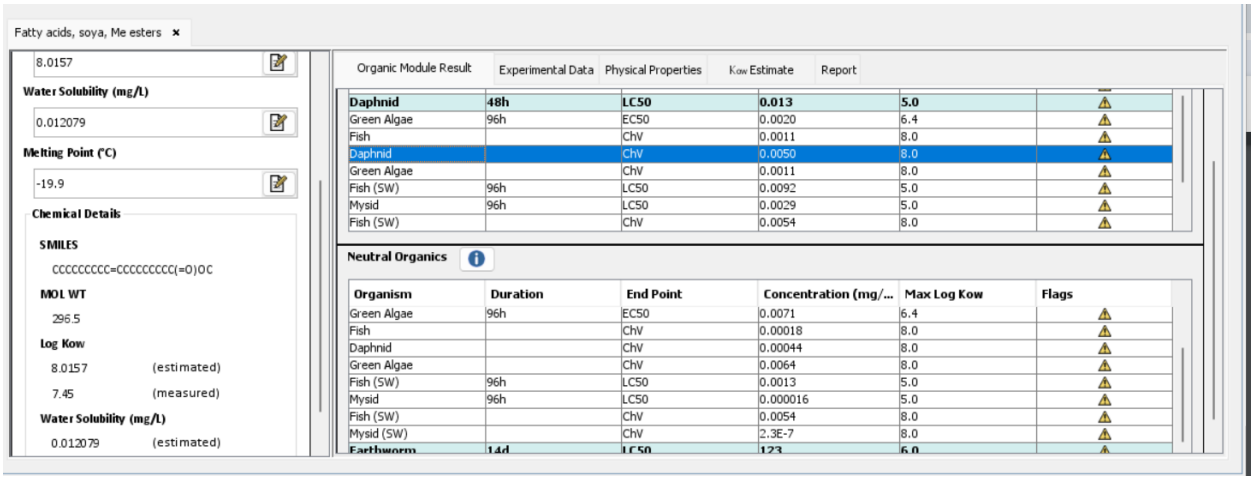
No discussions have been posted yet.

Ask a question about this chemical in the forums >

APPENDIX D: OECD Toolbox Respiratory Sensitization Results for Surrogate Methyl Oleate (CAS #112-62-9)



APPENDIX F: ECOSAR Modeling Results for Methyl soyate (CAS #68919-53-9)



APPENDIX G: EPI Suite™ Modeling Results for Methyl soyate (CAS #68919-53-9)

(Estimated values included in the GreenScreen® are highlighted and bolded)

CAS Number: 68919-53-9
SMILES : CCCCCCCCC=CCCCCCCCC(=O)OC
CHEM : Fatty acids, soya, Me esters
MOL FOR: C19 H36 O2
MOL WT : 296.50
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : 352.00
Melting Point (deg C) : 0.10
Vapor Pressure (mm Hg) : 3.12
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.69 estimate) = 8.02
Log Kow (Exper. database match) = 7.45
Exper. Ref: KROP,HB ET AL. (1997)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 352.56 (Adapted Stein & Brown method)
Melting Pt (deg C): 80.09 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.000118 (Modified Grain method)
VP (Pa, 25 deg C) : 0.0158 (Modified Grain method)
MP (exp database): -19.9 deg C
BP (exp database): 218.5 @ 20 mm Hg deg C
VP (exp database): 6.29E-06 mm Hg (8.39E-004 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 0.01208
log Kow used: 7.45 (expkow database)
melt pt used: 0.10 deg C

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.0025525 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Esters

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 1.44E-002 atm-m3/mole (1.45E+003 Pa-m3/mole)
Group Method: 7.73E-003 atm-m3/mole (7.84E+002 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.008E+002 atm-m3/mole (1.021E+007 Pa-m3/mole)
VP: 3.12 mm Hg (source: User-Entered)
WS: 0.0121 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 7.45 (exp database)
Log Kaw used: -0.230 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 7.680
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.8890
Biowin2 (Non-Linear Model) : 0.9912
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.9825 (weeks)
Biowin4 (Primary Survey Model) : 3.9180 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.7443
Biowin6 (MITI Non-Linear Model): 0.8436
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.7479
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 416 Pa (3.12 mm Hg)
Log Koa (Koawin est): 7.680
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 7.21E-009
Octanol/air (Koa) model: 1.17E-005
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 2.6E-007
Mackay model : 5.77E-007
Octanol/air (Koa) model: 0.000939

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 74.7180 E-12 cm3/molecule-sec [Cis-isomer]
OVERALL OH Rate Constant = 82.3180 E-12 cm3/molecule-sec [Trans-isomer]
Half-Life = 1.718 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
Half-Life = 1.559 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
Ozone Reaction:
OVERALL Ozone Rate Constant = 13.000000 E-17 cm3/molecule-sec [Cis-]
OVERALL Ozone Rate Constant = 20.000000 E-17 cm3/molecule-sec [Trans-]
Half-Life = 2.116 Hrs (at 7E11 mol/cm3) [Cis-isomer]
Half-Life = 1.375 Hrs (at 7E11 mol/cm3) [Trans-isomer]

Reaction With Nitrate Radicals May Be Important!
Fraction sorbed to airborne particulates (phi):
4.19E-007 (Junge-Pankow, Mackay avg)
0.000939 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 4.747E+004 L/kg (MCI method)
Log Koc: 4.676 (MCI method)
Koc : 9.557E+004 L/kg (Kow method)
Log Koc: 4.980 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Total Kb for pH > 8 at 25 deg C : 3.016E-002 L/mol-sec
Kb Half-Life at pH 8: 266.000 days
Kb Half-Life at pH 7: 7.283 years
(Total Kb applies only to esters, carbmates, alkyl halides)

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 3.307 (BCF = 2028 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.2924 days (HL = 1.961 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.071 (BCF = 117.8)
Log BAF Arnot-Gobas method (upper trophic) = 2.700 (BAF = 500.6)
log Kow used: 7.45 (expkow database)

Volatilization from Water:
Henry LC: 0.00773 atm-m3/mole (estimated by Group SAR Method)
Half-Life from Model River: 1.888 hours
Half-Life from Model Lake : 165 hours (6.874 days)

Removal In Wastewater Treatment:
Total removal: 94.00 percent
Total biodegradation: 0.78 percent
Total sludge adsorption: 93.02 percent
Total to Air: 0.21 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)
** Note: When the Log Kow is > 7, the model may be underestimating the mass of material in sediment and overestimating the mass of material in the water column (biota). Consider using the results of the default EQC model. **

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.168	1.31	1000
Water	17.7	360	1000
Soil	72.1	720	1000
Sediment	10.1	3.24e+003	0

Persistence Time: 467 hr

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.168	1.31	1000
Water	17.7	360	1000
water	(7.14)		
biota	(10.1)		
suspended sediment	(0.508)		
Soil	72.1	720	1000
Sediment	10.1	3.24e+003	0

Persistence Time: 467 hr

Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	**Half-Life (hr)**	**Emissions (kg/hr)**
Air	**0.0521**	**1.31**	**1000**
Water	**3.9**	**360**	**1000**
water	**(0.197)**		
biota	**(0.278)**		
suspended sediment	**(3.42)**		
Soil	**28.7**	**720**	**1000**
Sediment	**67.4**	**3.24e+003**	**0**

Persistence Time: 1.21e+003 hr

APPENDIX E: Change in Benchmark Score

Table 5 provides a summary of changes to the GreenScreen® Benchmark™ for methyl soyate. The original GreenScreen® assessment was performed in 2024 under version v. 1.4 criteria and ToxServices assigned a Benchmark 3 (BM-3a,3c) score.

Table 5: Change in GreenScreen® Benchmark™ for Methyl soyate

Date	GreenScreen® Benchmark™	GreenScreen® Version	Comment
December 3, 2024	BM-3a,3c	v. 1.4	Original GreenScreen® assessment.

Licensed GreenScreen® Profilers

Methyl soyate GreenScreen® Evaluation Prepared by:

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Methyl soyate GreenScreen® Evaluation QC'd by:

SIGNATURE BLOCK

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