

Dortmund Data Bank (DDB)

Biodiesel Related Data



Status of 2011-May-02

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 (0) 441 361819 0

Fax: +49 (0) 441 361819 10

E-Mail: support@ddbst.com

Web: www.ddbst.com

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Biodiesel

Biodiesel is a replacement fuel for petroleum-based diesel. Biodiesel is obtained from agricultural sources like oil seeds and counts therefore as a renewable energy.

Its main components are fatty acids methyl esters (FAME), ethyl esters, and mono-, di-, and triglycerides and the production process (transesterification) uses methanol or ethanol and produces glycerol. Additional reactive components are sodium and potassium hydroxide and the sodium and potassium alcoholates of methanol and ethanol.

Data Bank Content

The Dortmund Data Bank (DDB) contains for mixtures

- phase equilibrium information (vapor-liquid, liquid-liquid, solid-liquid),
- heats of mixing,
- densities, volumes, excess volumes,
- limiting activity coefficients,
- adsorbent/adsorptive equilibria,
- critical data
- Octanol/Water partition coefficients
- transport properties like viscosities

and several data for polymers. For pure components the DDB contains

- phase equilibrium information (vapor pressures, melting and boiling points, heats of vaporization, sublimation, and fusion, etc.)
- caloric data (heat of formation and combustion, heat capacities c_p and c_v , etc.)
- transport properties (viscosities, thermal conductivities)
- speed of sound
- P-v-T data (also virial coefficients)

Important Note

The following tables are not covering the complete content of the DDB because it only summarizes information on specific **pure** components and their mixtures. The Dortmund Data Bank also contains some data on biodiesel related components which are not entirely pure but a mixture of fatty acid esters – these “components” are mostly called pseudo-components. If the composition of these “components” is not given, the measured properties are maybe less useful.

Available Pure Component Data

Property	Compounds	References	Sets	Points
Dynamic Viscosity	69	63	213	725
Vapor Pressure	147	176	471	2390
Critical Data	17	15	40	40
Triple Point	6	4	6	6
Kinematic Viscosity	42	11	73	258
Density	130	210	670	3248
Melting Point	186	74	483	531
Molar Heat Capacity (cP)	40	21	107	1942
Heat of Vaporization	68	32	172	385
Heat of Fusion	31	14	58	78
Thermal Conductivity	10	12	66	1278
Surface Tension	72	33	152	601
Entropy	2	2	3	38
Std. Heat of Combustion	34	13	39	39
Std. Heat of Formation	30	12	44	44
Enthalpy (H-H0)	3	3	13	247
Gibbs Energy of Form.	1	1	1	1
Enthalpy (H-H0)/T	1	1	2	45
Transition Temperature	10	3	20	94
Heat of Transition	2	1	2	32
Dielectric Constant	25	16	36	95
Speed of Sound	13	15	27	145
Flash Point	1	1	1	1
Molar Saturation Heat Capacity	1	1	3	39
Heat of Sublimation	12	1	12	12
Thermal Expansion Coefficient	2	1	2	8
Total	316	473	2716	12322

Available Mixture Properties

The tables show all the available data for system containing at least one fatty acid ester.

Databank	Sets	Points	References
Activity coefficients at infinite dilution (ternary systems)	75	297	1
Activity coefficients at infinite dilution (binary systems)	768	768	40
Azeotropic/zeotropic information	746	746	136
Excess heat capacities	5	49	2
Critical data of mixtures	13	169	6
Vapor-liquid equilibria for systems containing solved salts	5	41	2
Salt solubilities	5	23	1
Gas solubilities	204	618	18
Heats of mixing	502	8269	65
Vapor-liquid equilibria (normal boiling point of a component below 0 °C)	453	4165	58
Liquid-liquid equilibria	379	3273	87
Thermodynamic data for polymer containing systems	55	420	15
Octanol-Water partition coefficients	36	36	10
Solid-liquid equilibria for systems without salts	410	2543	46
Densities and (excess) volumes of mixtures	928	12947	105
Mixture viscosities	200	2605	20
Vapor-liquid equilibria (normal boiling points of all components above 0 °C)	286	4510	112
Sum	5070	41479	(724)

The following table shows the amount of available data for fatty acid ester with either Methanol, Ethanol, or Glycerol.

Databank	Sets	Points	References
Activity coefficients at infinite dilution (binary systems)	33	33	5
Azeotropic/zeotropic information	85	85	33
Excess heat capacities	2	20	1
Heats of mixing	14	238	4
Liquid-liquid equilibria	5	57	2
Solid-liquid equilibria for systems without salts	6	16	1
Densities and (excess) volumes of mixtures	32	428	12
Mixture viscosities	38	542	6
Vapor-liquid equilibria (normal boiling points of all components above 0 °C)	67	962	29

Databank	Sets	Points	References
Sum	282	2381	(93)

Appendix

List of Methyl and Ethyl Esters

#DDB	Name	CAS-RN	Formula
248	Tetradecanoic acid methyl ester	124-10-7	C ₁₅ H ₃₀ O ₂
253	Hexadecanoic acid methyl ester	112-39-0	C ₁₇ H ₃₄ O ₂
262	Methacrylic acid methyl ester	80-62-6	C ₅ H ₈ O ₂
318	2-Propenoic acid ethyl ester	140-88-5	C ₅ H ₈ O ₂
340	(Z,Z)-9,12-Octadecadienoic acid methyl ester	112-63-0	C ₁₉ H ₃₄ O ₂
348	Dodecanoic acid methyl ester	111-82-0	C ₁₃ H ₂₆ O ₂
349	Octadecanoic acid methyl ester	112-61-8	C ₁₉ H ₃₈ O ₂
371	Ethyl butyrate	105-54-4	C ₆ H ₁₂ O ₂
405	Hexanoic acid methyl ester	106-70-7	C ₇ H ₁₄ O ₂
406	Octanoic acid methyl ester	111-11-5	C ₉ H ₁₈ O ₂
407	Decanoic acid methyl ester	110-42-9	C ₁₁ H ₂₂ O ₂
465	2-Propenoic acid methyl ester	96-33-3	C ₄ H ₆ O ₂
618	Ethyl 3-methylbutyrate	108-64-5	C ₇ H ₁₄ O ₂
635	Methyl oleate	112-62-9	C ₁₉ H ₃₆ O ₂
720	Methyl butanoate	623-42-7	C ₅ H ₁₀ O ₂
896	Methyl pentanoate	624-24-8	C ₆ H ₁₂ O ₂
897	Ethyl valerate	539-82-2	C ₇ H ₁₄ O ₂
1250	Octadecanoic acid ethyl ester	111-61-5	C ₂₀ H ₄₀ O ₂
1450	2-Methoxyfuran	25414-22-6	C ₅ H ₆ O ₂
1745	Cyclohexanecarboxylic acid,methyl ester	4630-82-4	C ₈ H ₁₄ O ₂
1762	Octanoic acid ethyl ester	106-32-1	C ₁₀ H ₂₀ O ₂
1836	Cyclohexene-4-carboxylic acid,methyl ester	6493-77-2	C ₈ H ₁₂ O ₂
2109	Nonanoic acid,methyl ester	1731-84-6	C ₁₀ H ₂₀ O ₂
2134	2-Methylpropanoic acid methyl ester	547-63-7	C ₅ H ₁₀ O ₂
2185	Hexanoic acid ethyl ester	123-66-0	C ₈ H ₁₆ O ₂
2307	Ethyl isobutyrate	97-62-1	C ₆ H ₁₂ O ₂
2310	Methyl isovalerate	556-24-1	C ₆ H ₁₂ O ₂

#DDB	Name	CAS-RN	Formula
2472	Ethyl heptanoate	106-30-9	C ₉ H ₁₈ O ₂
2473	Nonanoic acid ethyl ester	123-29-5	C ₁₁ H ₂₂ O ₂
2476	Methyl heptanoate	106-73-0	C ₈ H ₁₆ O ₂
2639	Ethyl methacrylate	97-63-2	C ₆ H ₁₀ O ₂
2655	trans-Chrysanthemic acid methyl ester	24141-52-4	C ₁₁ H ₁₈ O ₂
2837	Methyl undecanoate	1731-86-8	C ₁₂ H ₂₄ O ₂
2838	Tridecanoic acid methyl ester	1731-88-0	C ₁₄ H ₂₈ O ₂
2839	Methyl pentadecanoate	7132-64-1	C ₁₆ H ₃₂ O ₂
3053	Dodecanoic acid ethyl ester	106-33-2	C ₁₄ H ₂₈ O ₂
3076	Nonadecanoic acid methyl ester	1731-94-8	C ₂₀ H ₄₀ O ₂
3116	2-Methylbutanoic acid ethyl ester	7452-79-1	C ₇ H ₁₄ O ₂
3188	Heptadecanoic acid ethyl ester	14010-23-2	C ₁₉ H ₃₈ O ₂
3312	Tetradecanoic acid ethyl ester	124-06-1	C ₁₆ H ₃₂ O ₂
3313	Hexadecanoic acid ethyl ester	628-97-7	C ₁₈ H ₃₆ O ₂
3505	(Z)-9-Octadecenoic acid ethyl ester	111-62-6	C ₂₀ H ₃₈ O ₂
4101	Methyl 2,2-dimethylpropanoate	598-98-1	C ₆ H ₁₂ O ₂
4627	Adamantane-1-carboxylic acid methyl ester	711-01-3	C ₁₂ H ₁₈ O ₂
4680	Decanoic acid ethyl ester	110-38-3	C ₁₂ H ₂₄ O ₂
4790	2,2-Dimethylpropanoic acid ethyl ester	3938-95-2	C ₇ H ₁₄ O ₂
5323	(Z,Z,Z)-9,12,15-Octadecatrienoic acid methyl ester	301-00-8	C ₁₉ H ₃₂ O ₂
6113	2,8-Decadiene-4,6-dienoic acid methyl ester	505-02-2	C ₁₁ H ₁₀ O ₂
6114	2-Decene-4,6,8-trienoic acid methyl ester	7329-73-9	C ₁₁ H ₈ O ₂
6223	trans-2-Butenoic acid ethyl ester	623-70-1	C ₆ H ₁₀ O ₂
6224	trans-2-Butenoic acid methyl ester	623-43-8	C ₅ H ₈ O ₂
6237	Ethyl ester 10-undecenoic acid	692-86-4	C ₁₃ H ₂₄ O ₂
6238	Methyl undec-10-enoate	111-81-9	C ₁₂ H ₂₂ O ₂
6239	Ethyl ester 3-butenic acid	1617-18-1	C ₆ H ₁₀ O ₂
6470	(Z,Z)-9,12-Octadecadienoic acid ethyl ester	544-35-4	C ₂₀ H ₃₆ O ₂
7088	Eicosanoic acid methyl ester	1120-28-1	C ₂₁ H ₄₂ O ₂
7169	Methyl ester 4-pentynoic acid	21565-82-2	C ₆ H ₈ O ₂
7170	Ethyl ester 4-pentynoic acid	63093-41-4	C ₇ H ₁₀ O ₂
7171	Methyl ester 10-undecynoic acid	2777-66-4	C ₁₂ H ₂₀ O ₂

#DDB	Name	CAS-RN	Formula
7172	Ethyl ester 10-undecynoic acid	94030-75-8	C ₁₃ H ₂₂ O ₂
7173	Undecanoic acid ethyl ester	627-90-7	C ₁₃ H ₂₆ O ₂
7336	(Z)-6-Octadecenoic acid methyl ester	2777-58-4	C ₁₉ H ₃₆ O ₂
7337	(E)-6-Octadecenoic acid methyl ester	14620-36-1	C ₁₉ H ₃₆ O ₂
7338	(E)-9-Octadecenoic acid methyl ester	1937-62-8	C ₁₉ H ₃₆ O ₂
7339	(Z)-6-Octadecenoic acid ethyl ester	34302-52-8	C ₂₀ H ₃₈ O ₂
7340	(E)-6-Octadecenoic acid ethyl ester	34302-53-9	C ₂₀ H ₃₈ O ₂
7341	(E)-9-Octadecenoic acid ethyl ester	6114-18-7	C ₂₀ H ₃₈ O ₂
7732	3-Pentenoic acid methyl ester <Isomer not spec.>	818-58-6	C ₆ H ₁₀ O ₂
7797	2-Methyl butanoic acid methyl ester	868-57-5	C ₆ H ₁₂ O ₂
8038	Methyl ester 3-butenoic acid	3724-55-8	C ₅ H ₈ O ₂
9523	Ethyl 2,4-pentadienoate	13038-12-5	C ₇ H ₁₀ O ₂
9524	Ethyl cis-2-pentenoate	27805-84-1	C ₇ H ₁₂ O ₂
9525	Ethyl trans-2-pentenoate	24410-84-2	C ₇ H ₁₂ O ₂
9526	Ethyl cis-3-pentenoate	27829-70-5	C ₇ H ₁₂ O ₂
9527	Ethyl trans-3-pentenoate	3724-66-1	C ₇ H ₁₂ O ₂
9528	Ethyl 4-pentenoate	1968-40-7	C ₇ H ₁₂ O ₂
9530	Ethyl 3-pentynoate	52750-56-8	C ₇ H ₁₀ O ₂
10110	trans-2-Pentenoic acid methyl ester	15790-88-2	C ₆ H ₁₀ O ₂
10491	Heptadecanoic acid methyl ester	1731-92-6	C ₁₈ H ₃₆ O ₂
11098	cis-5,8,11,14,17-Eicosapentaenoic acid ethyl ester	86227-47-6	C ₂₂ H ₃₄ O ₂
11099	cis-4,7,10,13,16,19-Docosahexaenoic acid ethyl ester	84494-72-4	C ₂₄ H ₃₆ O ₂
11197	3,3-Dimethyl acrylic acid ethyl ester	638-10-8	C ₇ H ₁₂ O ₂
11308	Methyl 2-ethyl heptanoate	816-63-7	C ₁₀ H ₂₀ O ₂
11400	Docosanoic acid, methyl ester	929-77-1	C ₂₃ H ₄₆ O ₂
11401	Docosanoic acid, ethyl ester	5908-87-2	C ₂₄ H ₄₈ O ₂
11402	Tetracosanoic acid, methyl ester	2442-49-1	C ₂₅ H ₅₀ O ₂
11403	Hexacosanoic acid, methyl ester	5802-82-4	C ₂₇ H ₅₄ O ₂
11404	Hexacosanoic acid, ethyl ester	29030-81-7	C ₂₈ H ₅₆ O ₂
11405	Nonadecanoic acid ethyl ester	18281-04-4	C ₂₁ H ₄₂ O ₂
11406	Heneicosanoic acid, methyl ester	6064-90-0	C ₂₂ H ₄₄ O ₂
11407	Heneicosanoic acid, ethyl ester	28898-67-1	C ₂₃ H ₄₆ O ₂

#DDB	Name	CAS-RN	Formula
11408	Tricosanoic acid, methyl ester	2433-97-8	C ₂₄ H ₄₈ O ₂
11409	Tricosanoic acid, ethyl ester	18281-07-7	C ₂₅ H ₅₀ O ₂
11411	Octacosanoic acid, methyl ester	55682-92-3	C ₂₉ H ₅₈ O ₂
11412	Octacosanoic acid, ethyl ester	6624-78-8	C ₃₀ H ₆₀ O ₂
11413	Pentacosanoic acid, methyl ester	55373-89-2	C ₂₆ H ₅₂ O ₂
11414	Pentacosanoic acid, ethyl ester	29030-80-6	C ₂₇ H ₅₄ O ₂
11416	Nonacosanoic acid, methyl ester	4082-55-7	C ₃₀ H ₆₀ O ₂
11417	Nonacosanoic acid, ethyl ester	96591-06-9	C ₃₁ H ₆₂ O ₂
11418	Eicosanoic acid, ethyl ester	18281-05-5	C ₂₂ H ₄₄ O ₂
11848	Triacontanoic acid methyl ester	629-83-4	C ₃₁ H ₆₂ O ₂
11849	Triacontanoic acid ethyl ester	7505-12-6	C ₃₂ H ₆₄ O ₂
11851	Dotriacontanoic acid methyl ester	41755-79-7	C ₃₃ H ₆₆ O ₂
11852	Dotriacontanoic acid ethyl ester	29030-82-8	C ₃₄ H ₆₈ O ₂
11854	Tetracontanoic acid methyl ester	77630-49-0	C ₃₅ H ₇₀ O ₂
11855	Tetracontanoic acid ethyl ester	40952-09-8	C ₃₆ H ₇₂ O ₂
11857	Hexatriacontanoic acid methyl ester	88265-61-6	C ₃₇ H ₇₄ O ₂
11858	Hexatriacontanoic acid ethyl ester	76651-57-5	C ₃₈ H ₇₆ O ₂
11860	Octatriacontanoic acid methyl ester	129047-84-3	C ₃₉ H ₇₈ O ₂
11960	3-Pentenoic acid ethyl ester	1617-05-6	C ₇ H ₁₂ O ₂
11962	2-Pentenoic acid ethyl ester	2445-93-4	C ₇ H ₁₂ O ₂
12136	3,3-Dimethylbutanoic acid methyl ester	10250-48-3	C ₇ H ₁₄ O ₂
12150	2,4,4-Trimethylpentanoic acid methyl ester	64198-22-7	C ₉ H ₁₈ O ₂
12441	Ethyl ester 2-pentynoic acid	55314-57-3	C ₇ H ₁₀ O ₂
13624	Isolaurolic acid methylester	1460-88-4	C ₁₀ H ₁₆ O ₂
13625	Isolaurolic acid ethyl ester		C ₁₁ H ₁₈ O ₂
13626	Trimethylacrylic acid ethylester	13979-28-7	C ₈ H ₁₄ O ₂
13636	2-Butenoic acid ethyl ester <Isomer not specifi>	10544-63-5	C ₆ H ₁₀ O ₂
14688	Methyl 2,3,3-trimethylbutyrate	19910-30-6	C ₈ H ₁₆ O ₂
14689	Methyl 2-ethyl-2-methylbutyrate	5296-70-8	C ₈ H ₁₆ O ₂
14776	Bornylencarbonic acid ethyl ester		C ₁₃ H ₂₀ O ₂
14999	3-Methyl-2,4-hexadiene ethylester	72006-10-1	C ₉ H ₁₄ O ₂
15000	2,3-Dimethyl-2,4-hexadiene ethylester	103263-09-8	C ₁₀ H ₁₆ O ₂

#DDB	Name	CAS-RN	Formula
15001	3-Methyl-2-ethyl-2,4-hexadiene ethylester	100052-95-7	C ₁₁ H ₁₈ O ₂
15002	3,4-Dimethyl-2,4-hexadiene ethylester	103261-42-3	C ₁₀ H ₁₆ O ₂
15003	2,3,4-Trimethyl-2,4-hexadiene ethylester		C ₁₁ H ₁₈ O ₂
15004	3,4-Dimethyl-2-ethyl-2,4-hexadiene ethylester	105540-78-1	C ₁₂ H ₂₀ O ₂
15005	3,5-Dimethyl-2,4-hexadiene ethylester	91057-21-5	C ₁₀ H ₁₆ O ₂
15006	2,3,5-Trimethyl-2,4-hexadiene ethylester	59528-64-2	C ₁₁ H ₁₈ O ₂
15007	3,5-Dimethyl-2-ethyl-2,4-hexadiene ethylester	105539-91-1	C ₁₂ H ₂₀ O ₂
15014	Methyl erucate	1120-34-9	C ₂₃ H ₄₄ O ₂
16543	Ethyl 2-ethylbutyrate	2983-38-2	C ₈ H ₁₆ O ₂
16544	Ethyl 2,2-dimethylbutyrate	5129-40-8	C ₈ H ₁₆ O ₂
16545	Ethyl 3,3-dimethylbutyrate	5340-78-3	C ₈ H ₁₆ O ₂
16560	Propyneoic acid ethylester	623-47-2	C ₅ H ₆ O ₂
17449	Tridecanoic acid ethyl ester	28267-29-0	C ₁₅ H ₃₀ O ₂
19312	alpha-Methyl-beta-Propyl acrylic acid ethyl ester		C ₉ H ₁₆ O ₂
19313	alpha-Ethyl-beta-Propyl acrylic acid ethyl ester		C ₁₀ H ₁₈ O ₂
19314	alpha-,beta-Dipropyl acrylic acid ethyl ester		C ₁₁ H ₂₀ O ₂
19315	alpha-i-Propyl-beta-Propyl acrylic acid ethyl ester		C ₁₁ H ₂₀ O ₂
19316	alpha-Butyl-beta-Propyl acrylic acid ethyl ester		C ₁₂ H ₂₂ O ₂
20662	Heptacosanic acid, methyl ester	55682-91-2	C ₂₈ H ₅₆ O ₂
21449	Dihydrocampholenic acid ethyl ester		C ₁₂ H ₂₂ O ₂
21869	Suberene acetic acid methyl ester		C ₁₀ H ₁₆ O ₂
21870	Suberene acetic acid ethyl ester		C ₁₁ H ₁₈ O ₂
22360	Pulegonic acid methyl ester		C ₁₁ H ₁₈ O ₂
22552	5-Hexenoic acid methyl ester	2396-80-7	C ₇ H ₁₂ O ₂
23080	Methylpropyl acetic acid methyl ester		C ₇ H ₁₄ O ₂
23081	Methylpropyl acetic acid ethyl ester		C ₈ H ₁₆ O ₂
23084	Diethylacetic acid methyl ester		C ₇ H ₁₄ O ₂
23086	Ethylpropylacetic acid methyl ester		C ₈ H ₁₆ O ₂
23087	Ethylpropylacetic acid ethyl ester		C ₉ H ₁₈ O ₂
23089	Dipropylacetic acid methyl ester		C ₉ H ₁₈ O ₂
23090	Dipropylacetic acid ethyl ester		C ₁₀ H ₂₀ O ₂
24271	Ethyl trans-2-cis-4-decandienoate	3025-30-7	C ₁₂ H ₂₀ O ₂

#DDB	Name	CAS-RN	Formula
26698	(all-Z)-5,8,11,14,17-Eicosapentaenoic acid methyl ester		C ₂₁ H ₃₂ O ₂
26699	Methyl-cis-9-tetradecenoate	56219-06-8	C ₁₅ H ₂₈ O ₂
26700	Methyl-cis-10-pentadecenoate		C ₁₆ H ₃₀ O ₂
26701	Methyl-cis-9-hexadecenoate	1120-25-8	C ₁₇ H ₃₂ O ₂
26702	Methyl-cis-10-heptadecenoate		C ₁₈ H ₃₄ O ₂
26703	Methyl cis-11-eicosenoate		C ₂₁ H ₄₀ O ₂
26704	Methyl-cis,cis-11,14-eicosadieneoate		C ₂₁ H ₃₈ O ₂
26705	Methyl-cis,cis,cis-1,14,17-eicosatrieneoate		C ₂₁ H ₃₆ O ₂
26706	Methyl-(all-cis)-5,8,11,14-eicosatetraeneoate	2566-89-4	C ₂₁ H ₃₄ O ₂
26707	Methyl-cis,cis-13,16-docosadienoate		C ₂₃ H ₄₂ O ₂
26708	Methyl cis-15-tetracosenoate	2733-88-2	C ₂₅ H ₄₈ O ₂
26709	Methyl-(all-cis)-4,7,10,13,16,19-docosahexaeneoate		C ₂₃ H ₃₄ O ₂
27623	Ethyl trans-3-hexenoate	2396-83-0	C ₈ H ₁₄ O ₂
27631	Methyl 2-methylenenona-4-eneoate		C ₁₁ H ₁₈ O ₂
27632	Decadiene-(2,5)-1-carboxylic acid methyl ester		C ₁₁ H ₁₈ O ₂
27633	2-Methyl-pelargonic acid methyl ester		C ₁₁ H ₂₂ O ₂
27634	trans-Dec-2-enoic acid methyl ester	7367-85-3	C ₁₁ H ₂₀ O ₂
27635	cis-Dec-2-enoic acid methyl ester	75128-90-4	C ₁₁ H ₂₀ O ₂
27636	Dec-2-ynoic acid methyl ester		C ₁₁ H ₁₈ O ₂
27637	1-Methyl-1,4-pentadiene-4-carboxylic acid methyl ester		C ₈ H ₁₂ O ₂
27638	5-Methyl-2,5-hexadienoic acid methyl ester		C ₈ H ₁₂ O ₂
27639	5-Methyl hexanoic acid methyl ester	2177-83-5	C ₈ H ₁₆ O ₂
27640	Methyl 2-methyl-4-pentenoate		C ₇ H ₁₂ O ₂
27641	Methyl 2,4-dimethyl-4-pentenoate		C ₈ H ₁₄ O ₂
27642	5-Methyl-5-hexenoic acid methyl ester	32853-30-8	C ₈ H ₁₄ O ₂
27643	2,4-Dimethyl-pentanoic acid methyl ester		C ₈ H ₁₆ O ₂
27644	2-Methyl-4-decenoic acid methyl ester		C ₁₁ H ₂₀ O ₂
27645	Dec-5-enoic acid methyl ester		C ₁₁ H ₂₀ O ₂
27657	Methyl dec-9-enoate		C ₁₁ H ₂₀ O ₂
27658	trans-Methyl-dec-8-enoate		C ₁₁ H ₂₀ O ₂
27889	Methyl 4-pentenoate	818-57-5	C ₆ H ₁₀ O ₂
27948	Methyl 3-methylpentadecanoate		C ₁₇ H ₃₄ O ₂

#DDB	Name	CAS-RN	Formula
28037	Methyl undecylenate	5760-50-9	C ₁₂ H ₂₂ O ₂
28038	Methyl-5-heptenoate		C ₈ H ₁₄ O ₂
29265	Ethyl tetracosanoate	24634-95-5	C ₂₆ H ₅₂ O ₂
29272	Ethyl 2-butylhexanoate	2985-48-0	C ₁₂ H ₂₄ O ₂
29278	Ethyl 4-butyl-octylate		C ₁₄ H ₂₈ O ₂
29290	Ethyl 5-methylhexanoate	10236-10-9	C ₉ H ₁₈ O ₂
29297	Ethyl-7-methyl octanoate		C ₁₁ H ₂₂ O ₂
29309	Ethyl-6-methyl heptanoate		C ₁₀ H ₂₀ O ₂
29384	2-Ethylhexanoic acid ethyl ester	2983-37-1	C ₁₀ H ₂₀ O ₂
29387	3-Methylnonanoic acid ethyl ester		C ₁₂ H ₂₄ O ₂
29393	Ethyl 2-butyl-nonylate		C ₁₅ H ₃₀ O ₂
30235	Pentadecanoic acid ethyl ester	41114-00-5	C ₁₇ H ₃₄ O ₂

List of Glycerides

#DDB	Name	CAS-RN	Formula
603	Triolein	122-32-7	C ₅₇ H ₁₀₄ O ₆
615	Trilinolein	537-40-6	C ₅₇ H ₉₈ O ₆
631	Butanoic acid-1,2,3-propanetriyl ester	60-01-5	C ₁₅ H ₂₆ O ₆
1625	1,2,3-Propanetriol-triacetate	102-76-1	C ₉ H ₁₄ O ₆
3270	Hexanoic acid 1,2,3-propanetriyl ester	621-70-5	C ₂₁ H ₃₈ O ₆
3272	Decanoic acid 1,2,3-propanetriyl ester	621-71-6	C ₃₃ H ₆₂ O ₆
3273	Dodecanoic acid 1,2,3-propanetriyl ester	538-24-9	C ₃₉ H ₇₄ O ₆
3274	Tetradecanoic acid 1,2,3-propanetriyl ester	555-45-3	C ₄₅ H ₈₆ O ₆
3276	Hexadecanoic acid 1,2,3-propanetriyl ester	555-44-2	C ₅₁ H ₉₈ O ₆
3277	Octadecanoic acid 1,2,3-propanetriyl ester	555-43-1	C ₅₇ H ₁₁₀ O ₆
3398	Tripropionin	139-45-7	C ₁₂ H ₂₀ O ₆
9966	Octanoic acid, 1,2,3-propanetriyl ester	538-23-8	C ₂₇ H ₅₀ O ₆
10077	2,3-Bis(acetyloxy)propyl octadecanoate	33599-07-4	C ₂₅ H ₄₆ O ₆
14945	Triisopentylglycerol ester	620-63-3	C ₁₈ H ₃₂ O ₆
15072	Trilinolenin	14465-68-0	C ₅₇ H ₉₂ O ₆
17357	Heptanoic acid 1,2,3-propanetriylester	620-67-7	C ₂₄ H ₄₄ O ₆

21269	2,3-Acetoxypropyl propionate		C10H16O6
21317	Trielaidin	537-39-3	C57H104O6
21323	1-Oleoyl-2,3-dipalmitoylglycerol		C53H100O6
21324	1,3-Dipalmitoyl-2-oleoylglycerol	2190-25-2	C53H100O6
21325	1-Palmito-2-oleostearin		C55H104O6
21326	1-Palmito-2-stearo-olein		C55H104O6
21327	1-Oleo-2-palmitostearin		C55H104O6
21329	1,3-Dioleo-2-palmitin		C55H102O6
21330	1,2-Diaceto-3-olein		C25H44O6
21332	Tripelargonin		C30H56O6
21471	Tribenzoin	614-33-5	C24H20O6
22720	beta-Stearo-alpha,alpha-dilaurin		C45H86O6
22721	alpha-Stearo-alpha,beta-dilaurin		C45H86O6
22722	beta-Lauro-alpha,alpha-dimyristin		C43H82O6
22723	alpha-Lauro-alpha,beta-dimyristin		C43H82O6
22724	beta-Palmito-alpha, alpha-dimyristin		C47H90O6
22725	alpha-Palmito-alpha,beta-dimyristin		C47H90O6
22726	beta-Stearo-alpha,alpha-dipalmitin		C53H102O6
22727	alpha-Stearo-alpha,beta-dipalmitin		C53H102O6
22728	beta-Aceto-alpha,alpha-dipalmitin		C37H70O6
22729	alpha-aceto-alpha,beta-dipalmitin		C37H70O6
22730	beta-Capro-alpha,alpha-dipalmitin		C45H86O6
22731	alpha-Capro-alpha,beta-dipalmitin		C45H86O6
22732	beta-Lauro-alpha,alpha-dipalmitin		C47H90O6
22733	alpha-Lauro-alpha,beta-dipalmitin		C47H90O6
22734	beta-Myristo-alpha,alpha-dipalmitin		C49H94O6
22735	alpha-Myristo-alpha,beta-dipalmitin		C49H94O6
22736	beta-Aceto-alpha,alpha-distearin		C41H78O6
22737	alpha-Aceto-alpha,beta-distearin		C41H78O6
22738	alpha-Lauryl-alpha,beta-distearin		C51H98O6
23892	Tricrotonic acid glycerol ester		C15H20O6
26458	1-Stearyl-2-myristyl-3-palmitylglycerol		C51H98O6
26459	1-Stearyl-2-lauryl-3-palmitylglycerol		C49H94O6

26460	1-Stearyl-2-capryl-3-palmitylglycerol		C45H86O6
26461	1-Stearyl-2-palmityl-3-myristylglycerol		C51H98O6
26462	1-Stearyl-2-lauryl-3-myristylglycerol		C47H90O6
26463	1-Stearyl-2-capryl-3-myristylglycerol		C43H82O6
26464	1-Stearyl-2-palmityl-3-laurylglycerol		C49H94O6
26465	1-Stearyl-2-myristyl-3-laurylglycerol		C47H90O6
26466	1-Stearyl-2-capryl-3-laurylglycerol		C41H78O6
26467	1-Stearyl-2-palmityl-3-caprylglycerol		C45H86O6
26468	1-Stearyl-2-myristyl-3-caprylglycerol		C43H82O6
26469	1-Stearyl-2-lauryl-3-caprylglycerol		C41H78O6
27003	2-Benzoyl-1,3-di-p-nitrobenzoyl glycerol		C24H18N2O10
27007	2-Acetyl-1,3-di-p-nitrobenzoyl glycerol		C19H16N2O10
27692	Eicosanoic acid 1,2,3-propanetriyl ester	620-64-4	C63H122O6
27693	Docosanoic acid 1,2,3-propanetriyl ester	18641-57-1	C69H134O6
28575	1,3-Dibenzoyl-2-(p-nitrobenzoyl)glycerol		C24H19NO8
28583	1-(p-Nitrobenzoyl)-2,3-dibenzoyl glycerol		C24H19NO8
28591	1-Palmitoyloxy-2,3-dilauroyloxypropane		C43H82O6
28600	2-Capro-1,3-distearin		C49H94O6
28601	2-Lauro-1,3-distearin		C51H98O6
28602	2-Myristo-1,3-distearin		C53H102O6
28603	2-Palmito-1,3-distearin		C55H106O6
28604	1-Capro-2,3-distearin		C49H94O6
28605	1-Myristo-2,3-distearin		C53H102O6
28606	1-Palmito-2,3-distearin		C55H106O6
28607	1-Caproylo-2,3-distearin		C45H86O6
28608	1-Capryllo-2,3-distearin		C47H90O6
28609	2-Caproylo-1,3-distearin		C45H86O6
28610	2-Capryllo-1,3-distearin		C47H90O6
28650	9-Octadecenoic acid, 12-hydroxy-, 1,1',1''-(1,2,3-propanetriyl) ester, (9Z,9'Z,9''Z,12R,12'R,12''R)-	2540-54-7	C57H104O9
30323	Undecanoic acid 1,2,3-propanetriyl ester	13552-80-2	C36H68O6
30325	Tridecanoic acid 1,2,3-propanetriyl ester	26536-12-9	C42H80O6
30327	Pentadecanoic acid 1,2,3-propanetriyl ester	7370-46-9	C48H92O6
30328	Heptadecanoic acid 1,2,3-propanetriyl ester	2438-40-6	C54H104O6

30329	Nonadecanoic acid 1,2,3-propanetriyl ester	26536-13-0	C60H116O6
30330	Heneicosanoic acid 1,2,3-propanetriyl ester	26536-14-1	C66H128O6
30331	Tricosanoic acid 1,2,3-propanetriyl ester	86850-72-8	C72H140O6
30332	cis-9-Hexadecenoic acid 1,2,3-propanetriyl ester	20246-55-3	C51H92O6
30333	cis-6-Octadecenoic acid 1,2,3-propanetriyl ester	3296-43-3	C57H104O6
30334	cis-11-Octadecenoic acid 1,2,3-propanetriyl ester		C57H104O6
30336	cis-10-Nonadecenoic acid 1,2,3-propanetriyl ester		C60H110O6
30337	cis-11-Eicosenoic acid 1,2,3-propanetriyl ester		C63H116O6
30338	cis-12-Heneicosenoic acid 1,2,3-propanetriyl ester		C66H122O6
30339	cis-13-Docosenoic acid 1,2,3-propanetriyl ester	2752-99-0	C69H128O6
30340	cis-15-Tetracosenoic acid 1,2,3-propanetriyl ester	81913-24-8	C75H140O6
30502	Triazelain	20473-92-1	C30H50O12
31264	2,2-Dimethylpropionic acid 1,2,3-propanetriyl ester		C18H32O6
31265	n-Pentanoic acid 1,2,3-propanetriyl ester		C18H32O6
31266	i-Butyric acid 1,2,3-propanetriyl ester		C15H26O6
31620	trans-13-Docosenoic acid 1,2,3-propanetriyl ester		C69H128O6
31921	Tricyclobutylin		C15H20O6
31922	Tricyclo-valerine		C18H26O6
8119	1-Monostearin	123-94-4	C21H42O4
8120	1-Monopalmitin	542-44-9	C19H38O4
8121	1-Monomyristin	589-68-4	C17H34O4
8122	1-Monolaurin	142-18-7	C15H30O4
8123	1-Monocaprin	2277-23-8	C13H26O4
10103	2,3-Dihydroxypropyl ester 2-hydroxy benzoic acid	6170-45-2	C10H12O5
12429	Monoacetin	26446-35-5	C5H10O4
13524	Monoolein	111-03-5	C21H40O4
21048	.alpha.-Monoacetin	93713-40-7	C5H10O4
21147	Monopropionin		C6H12O4
21149	Monobutylin		C7H14O4
21248	Pentanoic acid, 2,3-dihydroxypropyl ester		C8H16O4
21249	Hexanoic acid, 2,3-dihydroxypropyl ester	502-53-4	C9H18O4
21250	Ricinoleic acid, 2,3-dihydroxypropyl ester		C21H40O5
21333	Isobutylin		C7H14O4

21334	Monovalerin		C8H16O4
21335	Monoisovalerin		C8H16O4
21336	Monocaproin (Isomer not specified)		C9H18O4
22807	1-Monooctanoin	26894-47-3	C11H22O4
22846	Glafenine	3820-67-5	C19H17CIN2O4
28584	1-Monobenzoylglycerol	3376-59-8	C10H12O4
28586	1-(p-Nitrobenzoyloxy)-2,3-dihydroxypropane		C10H11NO6
8113	2-Monostearin	621-61-4	C21H42O4
8114	2-Monopalmitin	23470-00-0	C19H38O4
8115	2-Monomyristin	3443-83-2	C17H34O4
8116	2-Monolaurin	1678-45-1	C15H30O4
8117	2-Monocaprin	3376-48-5	C13H26O4
8118	2-Monobenzoylglycerol	3376-49-6	C10H12O4
21049	.beta.-Monoacetin		C5H10O4
28574	2-(p-Nitrobenzoyl)glycerol		C10H11NO6
21045	1,2-Diacetin		C7H12O5
28567	1,2-Dibenzoylglycerol		C17H16O5
31618	Gyceryl dierucate	28880-79-7	C47H88O5
31619	Glyceryl dibrassidate		C47H88O5
10224	Acetic acid 3-acetoxy-2-hydroxypropyl ester	105-70-4	C7H12O5
10678	(3-Acetyloxypropyl) octadecanoate	820-17-7	C23H44O5
21331	1,3-Dipalmitin	502-52-3	C35H68O5
21630	1,3-Diolein	2465-32-9	C39H72O5
22717	1,3-Distearin	504-40-5	C39H76O5
22718	1,3-Dilaurin	539-93-5	C27H52O5
22719	1,3-Dimyristin	7770-09-4	C31H60O5
22804	Dibutyryne	32648-01-4	C11H20O5
28556	1,3-Dibenzoyloxy-2-propanol	40593-13-3	C17H16O5