Research Article

Fatty Acid Content in Biomasses: State-of-the-Art and Novel Physical Property Estimation Methods

Ana M. Sousa [ID],[1] **Thalles A. Andrade** [ID],[2] **Massimiliano Errico** [ID],[2] **José P. Coelho** [ID],[3,4] **Rui M. Filipe** [ID],[1,3] and **Henrique A. Matos** [ID][1]

[1]CERENA/DEQ, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, Lisboa, Portugal
[2]Department of Chemical Engineering, Biotechnology and Environmental Technology, University of Southern Denmark, Campusvej 55, 5230 Odense, Denmark
[3]Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, 1959-007 Lisboa, Portugal
[4]CQE, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, Lisboa, Portugal

Correspondence should be addressed to Massimiliano Errico; maer@kbm.sdu.dk

In line with the growing environmental awareness developed along the last decades, modern societies are urged to evolve into sustainable economics where the reuse of organic wastes represents the key feedstock for a green transaction. The oil phase obtained from different biomasses has the potential to be a source of food supplements, medicines, cosmetics, or feedstock for biofuel production. In the present work, the composition of 104 different biomasses including seeds, peels, flowers, plants, and leaves has been reviewed for the lipid content. Based on the most frequent fatty acids screened, experimental data for normal boiling point temperature, normal melting point, critical properties, and acentric factor were collected and compared with the most common estimation methods, which are functions of the molecular structure and interaction between different functional groups. New predictive equations have been proposed to reduce the estimation deviation and to provide simple correlations to be used in simulation software when dealing with biomass processes. For all the properties, the estimations proposed have an absolute average deviation equal to or lower than 4.6%.

1. Introduction

The development of sustainable processes can be pursued through multiple paths, among which decreasing wastes, increasing efficiency in industrial processes, mitigating environmental and human risks, reducing pollutant agents, and fostering energy production from renewable sources play unquestionable roles.

Within this context, biomass appears as a valuable feedstock to recover several compounds and/or produce energy to answer the global consumption growth without creating a negative legacy to the next generations [1]. In fact, the widespread employment of biomass not only bears the potential of recovering industrial wastes as a valuable resource but also leverages the energy and industrial productions through efficient and less polluting engineering processes.

This work is deemed to study the potential of fatty acids in addressing significant multidisciplinary issues associated with the chemical industry and petroleum exploration [2], incorporated in the broader research initiative aiming to develop integrated processes and product design for sustainable biorefineries [3].

Fatty acids are long hydrocarbon chains with a terminal carboxyl group. They can be obtained from rather abundant organic compounds, including organic matter wastes [4, 5] or nonedible oils [6, 7]. Fatty acids are characterized by an outstanding range of applications within the energy domain, such as biofuels [8], and flow improvers for crude oils [9–12], or within other high end industries such as food supplements [13], cosmetics [14], medicines, and drugs [15, 16].

Fatty acids, often referred to as fats, are used in the human body to store excess energy, and they constitute the building blocks for membrane cells [17, 18]. Moreover, as recommended by the Food and Agriculture Organization of the United Nations [19], there is convincing evidence that some fatty acids like the linoleic acid and the alpha-linoleic

acid are indispensable for human health even if they cannot be synthesized.

Considering the broad range of fatty acid applications, an extensive review of their amount and composition in different biomasses has been drawn.

Such remarkable potential opens the definition of new industrial processes for fatty acid recovery from different biomasses contributing to valorize poor feedstocks and to reduce their environmental impact when treated as wastes. Such approach paved the way in applying strategies deemed to foster sustainability on an industrial scale.

Within a biorefinery approach, the target compounds are recovered or obtained from the biomass through a series of processes classified as thermochemical, biochemical, mechanical/physical, and chemical [20]. It means that, in order to move from the definition of the biomass potential in recovering or obtaining some compounds to the process setup, a reliable model must be available to design the single unit operation and to define the process global performance and profitability. Product and process design rely on the knowledge of the properties of chemical compounds and their mixtures. Although large databases of experimental data are available, covering the complete set of compounds, mixtures, and operating conditions is a huge task that may not be economically feasible. Property estimation models for physical properties are widely used when experimental data are not available.

Unlike what can be found in published research concerning thermophysical properties of pure compounds, this work has been focused on the most important temperature-independent physical properties of the main fatty acids found in biomass feedstocks. These properties are also essential in improving the processes modeling, in the formulation of product portfolios and for the composition assessment of the generated pollutants.

Published prediction methods were critically analyzed given the scarcity of experimental data for determining the relevant physical properties. Considering current methods shortcomings for the intended applications and using the National Institute of Standards and Technology (NIST) database as a reference, innovative estimation methods were developed. Such correlation's novelty is not only limited to a higher accuracy but also finds a significant advantage in its simplicity, given the use of molecular weight (MW) and the maximum number of double bonds (DBs) in the molecule as input. To sum up, a reliable method for the estimation of fatty acid (FA) physical properties was developed. Therefore, a set of six new correlations have been proposed to reduce the estimation deviation of boiling point, melting point, critical properties, and acentric factor.

Such a tool will be of paramount importance in proposing strategies that congregate high-value addition in industrial processes with the use of abundant biomass and the reuse of potentially polluting waste from food or other related processes, such as the waste from olive oil or wine manufacture.

2. Review on Fatty Acid Content in Biomasses

A biorefining process is based on the usage of selected biomass(es) treated in a smaller or larger unit, locally or centrally, for the production of valuable final products or intermediates with applications in pharmaceutical, food and beverages, or even nutraceutical fields [21]. Subsequently, waste biomass effluents could be treated to produce lower added-value products, e.g., insecticides or pesticides, or used as feedstock for biofuel production.

A total of 104 different types of oils obtained by extraction of different biomasses were collected from the scientific literature to identify the most common and frequent fatty acids. The list of oil sources and main fatty acid composition is reviewed in Table 1. The information was collected and summarized from different published works, and when available, the minimum and maximum concentration values were reported. In some cases, the percentage of oil content in the biomass matrix was also included. This value could be useful to determine a possible upper bound oil extraction yield from the biomass matrix. In Table 1, 16 fatty acids were listed since, according to the sources reviewed, they appear in the oil in a significant amount.

Ricinoleic acid, lesquerolic acid, and elaeostearate acid, the main constituents of castor oil, lesquerella oil, and tung oil, respectively, were not reported since they do not appear in the other biomasses listed. Information about their quantity is provided in Table 1 notes.

Figure 1 shows the average of each fatty acid yield in the biomasses and their frequency of appearance.

The fatty acid yield average was obtained by considering the values reported in Table 1. For those cases where a yield interval is indicated, the average was calculated. The frequency of appearance expresses the occurrence of fatty acid in the set of biomasses.

Regarding the saturated fatty acids, palmitic acid (C16 : 0) and stearic acid (C18 : 0) are the ones with the highest content and frequency in all the bio-oils examined. Considering the unsaturated fatty acids, oleic acid (C18 : 1), linoleic acid (C18 : 2), and linolenic acid (C18 : 3) are the most plentiful compounds identified in the reported bio-oils. However, since the average yield reported in Figure 1 was evaluated considering the distribution of the single fatty acids, a more revealing indicator is the average minimum and average maximum, reported in Figure 2 as a grey rectangle. The minimum and maximum averages were published together with the absolute minimum and absolute maximum. On the one hand, taking caprylic acid as an example, its average yield range is from 0.2% to 5.2%, which is a very narrow range, while the absolute maximum is 11.4%. On the other hand, when palmitoleic acid, oleic acid, and linoleic acid are considered, their amount can extensively vary.

3. Fatty Acid Classification

Oil extracts from biomasses comprise saturated and unsaturated fatty acids with long carbon chain, which can be employed in integrated processes for sustainable biorefineries. To highlight the differences between the molecules, the different fatty acids were identified based on the number of carbon atoms (CN) and the number of carbon-carbon double bonds (DB).

TABLE 1: Fatty acid content in the selected biomasses expressed in weight.

Biomass	Oil content (%)	Caprylic acid, C8:0 (%)	Capric acid, C10:0 (%)	Lauric acid, C12:0 (%)	Myristic acid, C14:0 (%)	Palmitic acid, C16:0 (%)	Palmitoleic acid, C16:1 (%)	Stearic acid, C18:0 (%)	Oleic acid, C18:1 (%)	Linoleic acid, C18:2 (%)	α-Linolenic acid, C18:3 (%)	Arachidic acid, C20:0 (%)	Eicosenoic acid, C20:1 (%)	Eicosadienoic acid, C20:2 (%)	Behenic acid, C22:0 (%)	Erucic acid, C22:1 (%)	Lignoceric acid, C24:0 (%)	Others (%)	References
Alexandrian laurel (*Calophyllum inophyllum*)	NA					13.9	0.2	15.1	40.3	25.6	0.2	0.3							[22]
Almond	NA					5.07–6.78	0–0.5	0–1.4	57.54–73.94	19.32–35.18	0.04–0.10							0–0.9	[23, 24]
Andiroba (*Carapa guianensis*)	NA					27	1	7	49	16					0–0.2				[25]
Argemone mexicana	30–40					14.1–15.3	0–1.3	3.7–9.8	34.3–45.8	29.0–44.2	0–0.3	0–0.3							[26]
Avocado seeds	1.1–1.6	0–0.28		0.20–0.60	0–0.1	17.7–20.85	1.79–4.60	0.90–1.50	17.41–24.1	35.30–38.89	4.10–6.58	0.04–0.80	0.45–2.00		0.40–1.11	0–0.12		0–5	[27, 28]
Babassu kernel (*Orbignya* sp.)	60–70	0–5	0–6	35–48	13–16	9–10		2–4	14–17	2–5							1.68–3.30		[25, 29, 30]
Bay laurel fruit	NA				3.5	21.8	0.5	3.8	30.9	20.5	0.4							0.3	[31]
Bay laurel leaves	NA				4.5	25.5	0.3	3.1	10.6	11.3	17.1							1.4	[24, 31]
Bitter almond	NA				0.1	10.3		3.9	33.9	46.0	4.8	0.2							[32]
Black currant (*Ribes nigrum* L.)	2.2					6.4		1.6	16.1	57.8	13.2	0.2							[33]
Burdock seeds	15–20					7				69					4.7				[34]
Camelina	38–47				0.05–0.2	5.1–6.8	0–0.3	2.7–3.4	14.3–19.7	14.3–19.6	28.6–38.4	0.25–1.83	11.9–16.8	1.3–2.2	0.2–1.4	2.3–4.2	0–0.14	0–0.8	[35–38]
Carapa seeds	51					25.3	0.6	10.5	57.8	5.9									[39, 40]
Carob seeds	1.73–1.84				0.5	10.3–12.0	0.6	3.5–4.6	28.1–31.8	49.1–51.0	1.4–1.7	0–0.66	0.6					1.7–2.5	[41]
Castor oil	42–54					0.84–1.30		0.78–3.60	2.92–4.90	1.27–5.40	0–0.78	0–0.66	0–0.63					84.7–89.6[a]	[42–47]
Chia (*Salvia hispanica* L.)	25–38					5.5–8.9		2.7–4.8	5.3–8.4	15.7–26	50.0–69.3				0.8				[48–50]
Chokeberry (*Aronia melanocarpa* L.)	1.93					5.1		1.1	21.4	71.1	0.5								[33]
Chlorophyceae (*Botryococcus* sp.)	6.19					20.56	8.20	4.56	44.74	6.36	15.55								[51]
Chlorophyceae (*Chlorella* sp.)	14.05				1.60	0.86	35.72	0.85	8.53	21.50	15.30	0.36						15.27	[51]
Chlorophyceae (*Chlorococcum* sp.)	8.21				0.86	21.65	0.90	0.50	20.60	21.30	2.81	0.42	16.53					12.66	[51]
Chlorophyceae (*Dunaliella salina*)	6.25					36.40		5.30	50.81	7.46									[51]
Coconut (copra)	NA	8.0–8.9	6.0–6.2	47.0–48.8	17.0–19.9	7.8–9.7		3.0	4.4–7.0	0.8–2.2	0–0.48	0–0.24						0.3	[24, 42, 52]
Cottonseed	NA				0.67–3.45	11.67–11.80	0.42–4.05	1.85–2.00	24.80–25.16	60.60–61.30								0.3	[24, 42, 43]
Crambe abyssinica	35			0.26	0.20	8.83–28.70	0.1	0.89–14.72	10.3–30.7	20.6–62					0.80	58.51	1.12		[42, 43, 53–55]
Crataegus monogyna	NA					2.07		0.70	18.86	9.00	6.85	2.09	1.37		1.01				[43, 56, 57]
Cumaru (*Dipteryx odorata*)	NA					13.21		2.23	33.78	44.60									[58]
Cuphea viscosissima	NA	0.3	64.7			23		7	37	29								4	[25]
Cyanophyceae (*Calothrix* sp.)	3.42			3.0	4.5	7.0	6.55	0.9	12.2	6.7									[59]
Cyanophyceae (*Leptolyngbya* sp.)	3.23					26.95	1.53	3.99	55.52	5.36									[51]
Cyanophyceae (*Lyngbya* sp.)	2.52				1.23	13.74	5.37	4.73	69.52	4.00	1.56				3.57				[51]
Cyanophyceae (*Nostoc muscorum*)	3.22					26.49		3.24	54.53		5.15								[51]
Cyanophyceae (*Oscillatoria acuta*)	4.47				0.21	26.89	2.01	8.53	54.01	7.85	11.24								[51]
Cyanophyceae (*Oscillatoria martina*)	6.61					13.61	2.34	4.74	68.68	9.17					1.60				[51]
Cyanophyceae (*Spirulina platensis*)	7.75					18.74		5.21	63.15	7.74	1.94				5.52				[51]
Cyanophyceae (*Synechococcus* sp.)	4.2					22.53	82.12	1.73	53.54	5.45		0.65							[51]
Ethiopian mustard (*Brassica carinata*)	NA					8.74		1.0	9.7–33.9	8.2–16.8	1.1–16.6	0.7	10.9			42–42.5		9.6	[60–62]
Euphorbia lathyris L.	46					2.9–3.1	0–0.50	0–1.98	78.20–81.46	3.71–4.62	2.78–7.85		0–0.50			0–0.20			[63, 64]
Forsythia suspensa	30					5.53–6.80		1.99	18.68	72.89	0.79								[65]
Goji berry (*Lycium barbarum* L.)	NA					5.65	1.0–3.1	2.61–4.78	16.7–22.4	37.0–44.00	0–0.6	1.0–3.0			0.48–6.78				[66]
Grape seeds	NA				0–0.09	7.2–10.35	0–0.4	2.1–2.6	12.80–29.1	52.26–65.33	0.2	0–0.2	0–0.38		0–0.10				[58, 67]
Hazelnut kernel (*Corylus avellana*)	51–75					4.9–5.1		5.40–9.5	76.9–83.6	8.5–13.1	0–0.6	0–0.2	0–0.3					0–0.4	[24, 42, 68]
Jatropha curcas	50–60			0–0.31	0.30–3.50	13.23–14.9	0.85–0.88	5.40–9.5	40.5–45.79	32.27–36.99	0–0.3	0.30–3.80			0–0.10		1.40–4.40	0–1.93	[60, 64, 69, 70]
Jojoba (*Simmondsia Chinensis*)	45–55					3.10–9.00	0.60–2.20	11.11	28.20–46.30	0.20–3.10			20.80–51.50			0–14.5		0.50–19.70	[71–73]
Karanja (*Pongamia pinnata*)	30–40			0.31		7.4–11.6		4.1–6.5	51.6–65.6	15.4–16.6	0–4.4							3.4–12.7	[60, 70, 74]
Kusum (*Schleichera trijuga*)	NA				15.54	10.35		1.8	44.5–61.9	1.0–2.5		15.79	6.17	0.08				7.42	[75]
Lemon seeds	33.4–41.9					23.5–29.4		2.41–2.5	24.8–29.3	33.2–36.3	3.2–7.8	0.8	0.9					0.5–1.5	[76]
Lesquerella fendleri	NA				0.3	1.0	0.4	18.97–25.8	13.6	6.7	10.2							64.3[b]	[47]
Linseed	35–45					4.92–5.1	0.3	11.8	18.9–19.7	18.03–18.1	54.94–55.1								[42, 43, 60]
Mahua (*Madhuca indica*)	35–40				0–0.14	16.0–28.2	0.3	13.65–14.19	37.2–51.0	8.9–19.5	0–0.16	0.5				0.6			[60, 70, 77]
Meliaceae (*Aphanamixis polystachya*)	NA					18.4		4.6–6.8	18.3	26.7	23.2								[78]
Mesua ferrea seeds	55–57				0.05–2.13	10.85–13.64	0–0.09	9.0–10.50	50.71–55.93	13.68–19.47		0–1.3	0.2			0.6			[79–81]
Michela champaca	45.0–45.5				0–0.57	15.8–32.52	6.9–13.39	27.1–36.3	22.8–28.9	30.72–42.5	0–0.32	2.9–4.3	0–0.71		0–0.35		0–0.19		[82, 83]
Milk thistle	NA					7.3–8.4		1.51	30.3–47.2	49.7–53.6	0–0.3	0–0.6	0.8–0.9		2.3–2.9		0.6–0.8		[84]
Milkweed seed (*Calotropis gigantea*)	NA				0–0.1	6.5–13.8	1.1–2.0	14.2–24.1	72.1–36.3	1.0–2.5	0–0.8	3.8–4.0			2.3–2.9		0–0.4		[85]
Moringa seed	38–40				0.05	5.54	0.21	10.1	8.83	10.79	0–0.9	1.21	0.9–2.0		1.09		1.68	4.43	[86, 87]
Mustard seed	NA				0–0.26	5.54	0–0.2	1.6	44.5–61.9	2.3–18.3	20.98	0.8–3.4	5.27		0.01	37.71	1.68		[36]
Neem (*Guizotia abyssinia*)	20–30					13.6–18.1		2.68–3.00	44.5–61.9	10.79	0.2–3			0.70	1.09				[60, 88–91]
Olive kernel	30					9.2		10.1	9.0	71.7	9.0								[92]
Olive pomace	NA				0–0.04	5.0	0.3	4.1	74.7	17.6	17.6	0–0.58	0–0.40		0–0.22	0.6		0.8	[24, 42]
Opium poppy (*Papaver somniferum* L.)	8.5–14.9					9.37–16.20	0.68–0.80	2.68–3.00	69.3–79.0	7.20–12.70	0.30–0.87	0–0.58	0.18–2.92					1.7	[93–95]
Orange peel	NA					38.6	0.13	4.1	11.94	74.47		0–1.3	0–0.71					0.1	[96]
Palm (*Eliais* sp.)	NA		5.0	0–0.3	0–1.1	35–43	0–0.3	4–7	40–44	10–14	0–0.2	0–0.3	0.8–0.9		2.3–2.9		0.6–0.8	0–1.1	[25, 35, 42, 98]
Corozo palm/Macaiba (*Acrocomia aculeata*)	NA	5.0		50.9	13.1	7.6		3.0	17.9	2.5	2.5								[99]
Peanut (*Arachis hypogaea*)	40–50					6.7–11.4		1.73–3.99	47.06–78.2	4.4–32.0	0.19–0.93	0–3.0			2.52–3.93	0–0.73	1.23–1.83	0–0.1	[42, 43, 68, 100, 101]
Peppers (*Capsicum*)	NA				0–1.1	10.6–14.4	0–0.3	2.7–3.9	5.4–7.6	73.9–77.9	5.4–7.6	0–0.3							[102]
Pequi (*Caryocar* sp.)	NA					40		2	47	4			0–1.9					7	[25]

Table 1: Continued.

Biomass	Oil content (%)	Caprylic acid, C8:0 (%)	Capric acid, C10:0 (%)	Lauric acid, C12:0 (%)	Myristic acid, C14:0 (%)	Palmitic acid, C16:0 (%)	Palmitoleic acid, C16:1 (%)	Stearic acid, C18:0 (%)	Oleic acid, C18:1 (%)	Linoleic acid, C18:2 (%)	α-Linolenic acid, C18:3 (%)	Arachidic acid, C20:0 (%)	Eicosenoic acid, C20:1 (%)	Eicosadienoic acid, C20:2 (%)	Behenic acid, C22:0 (%)	Erucic acid, C22:1 (%)	Lignoceric acid, C24:0 (%)	Others (%)	References
Polanga (Calophyllum inophyllum)	NA					13.9	0.2	15.1	40.3	25.6	0.2	0.3						4.4	[22]
Poon (Sterculia foetida)	NA			0.1	0.2	18.4–23.0	0.3	7.3–8.2	1.0–16.4	11.0–45.9	0.7–2.3	2.3–6.5							[103, 104]
Poppy seed	49.9–52.4					8.2–12.6	0–0.1	0–4.0	13.3–23.4	60.2–74.3	0–0.5								[24, 105]
Pot marigold seeds (Calendula officinalis L.)	NA					3.86–4.55		0–2	4.44–6.25	28.50–31.86	51.47–57.63								[106]
Pumpkin seeds	45			0–0.01	0–0.11	10.2–12.51	0–0.15	5.43–6.0	36.1–37.07	43.72–45.2	0.18–2.6		0–0.39	0–0.11	0–0.12	0–0.02	0–0.06		[107, 108]
Putranjiva roxburghii	NA				0.03	10.23	0.07	10.63	48.65	27.50	0.87	1.05	0.30		0.24	0.03	0.31	0.09	[109]
Quinoa (Chenopodium quinoa)	NA				0.14–0.16	8.3–8.9		0.64–0.68	20.8–24.9	50.7–54.3	7.7–8.4	0.55–0.59	1.53–1.75	0.15–0.17	0.96–1.01	1.87–1.93	0.44–0.46		[110]
Rapeseed (Brassica napus) or canola oil	40–44				0–0.24	3.49–4.82	0–0.36	0.85–2.10	58.9–64.4	18.8–22.3	7.6–11.1	0–0.70	0–1.35		0–1.45	0–1.09	0–0.12	0–2.48	[35, 42, 43, 54, 63, 68, 69, 111, 112]
Rice bran (Oryza Sativa)	10–26				0.5	16.2		2.1	42.8	37.2	1.6	3.5						1.2	[113]
Rosehip seed (Rosa canina L.)	0.82			2.5	0.4	17.8	2.6	8.8	52.6	2.1	2.1				8.0				[33]
Rubber (Hevea brasiliensis) seed	35–60				0–2.2	0.23–10.6	0.23–0.25	5.69–12	12.7–42.08	39.6–52.84	2.38–26	0.66–0.97							[54, 114, 115]
Safflower seed	NA					7.3–8.6		1.9–1.93	11.58–13.6	77.2–77.89									[24, 42, 43]
Sapium sebiferum	NA					5.45	3.71	2.13	13.78	30.71	38.87		0.59					4.76	[64]
Sal (Shorea robusta) seed	10–12			0.58		3.69–8.6		34.2–47.0	34.2–44.8	1.2–2.7		3.5–12.2							[60, 116, 117]
Sea buckthorn leaves	NA				1.6	19.6	1.5	3.2	7.1	9.5	51.1				3.2			3.2	[118]
Sea buckthorn peels	NA				0.4	32.9	28.6	1.8	16.1	8.8	4.4							7.0	[118]
Sesame seeds	35–58					7.0–13.1	0.37	3.5–7.0	35.0–52.8	30.2–50.0	1.94							0.32	[24, 42, 43, 119–121]
Soapnut	18–22					4.67	0–0.3	1.45	52.64			7.02	23.85		1.45	1.09	0.47	0–6	[69]
Soybean (Glycine max)	NA					10–14		2–4.1	23–24.1	52–56.2	0–8								[25, 35, 36, 42, 43, 54, 68, 70, 98, 122]
Spruce bark	NA			0.25	0.87	11.91		3.00	1.25			8.65			34.22		35.60	4.3	[58]
Stillingia oil (Sapium sebiferum Roxb.)	13–32			3.55	0.31	5.93–7.72		2.05–2.46	15.24–15.93	29.05–29.77	39.54–41.20							1.75	[123, 124]
Sunflower seed	NA					6.08–6.8	0.1	2.9–3.26	16.93–17.7	72.9–73.73		0.19–0.21							[24, 43, 54]
Syringa (Melia azedarach L.)	NA					9.7–10.1		3.31–3.67	21.69–22.31	63.27–64.89	0.34–0.43		0–0.36						[125]
Tallow (animal fat)	NA					23.3	0.1	19.3	42.4	2.9	0.9							2.9	[24]
Tallow (Triadica sebifera L.)	NA					55.78		0.54	5.92	9.13	28.55							0.1	[126]
Terminalia catappa	NA				0–0.1	28.3–35.0	0–0.9	4.9–5.0	30.0–32.0	28.0–32.8	0–1.7	0.3–0.8							[39, 127]
Terminalia (Terminalia belerica Robx.) seed oil	31–43					11.6–32.8	0–0.5	3.9–6.4	31.3–61.5	18.5–28.8									[128–130]
Tiger nut (Cyperus esculentus)	78.69				1.7	15.4		5.3	65.8	5.5	0.2	6.1							[131]
Tobacco seed (Nicotiana tabacum L.)	38				0.09–0.17	3.0–10.96	0–0.20	3.34–5.0	12.14–16.0	67.75–72.98	0.69–4.20	0.20–0.25	0.12–0.13		0.07–0.12		0–0.04	0.69–3.12	[132–135]
Tung (Vernicia montana)	NA					2.3	0–0.2	2.4	5.6	6.3	0.1	0.2	0.9					82.2c	[136–140]
Walnut (Juglans regia)	52–70					7.2	1.0	1.9–2.6	15.1–18.5	56.0–60.7	12.8–16.2	0–0.2	0–0.2				0.1	0–0.5	[24, 42, 68, 141, 142]
Wheat germ	NA				0–0.13	17.4–18	0.17–0.23	0–0.7	16.5	55.1–57.7	7.9			0–0.28					[24]
Wheat grain	NA					20.6	1.0	1.1	16.6	56.0	2.9							1.8	[143]
Waste coffee ground	10–15	11.4			0.4	33.99		10.91	7.16	23.27		4.04						20.6	
Yellow oleander seed (Thevetia peruviana)	60–65					15.03–23.28	0–0.39	6.16–10.71	43.72–44.35	19.85–31.99	0–0.79	0.79–2.41			0–0.49				[144–146]
Zanthoxylum bungeanum	24–28					10.3	10.8	1.1	35.9	24.8	15.9							1.2	[147]

aCastor oil contains 89.6 ricinoleic acid. bLesquerella oil contains 57.6 lesquerolic acid. cTung oil contains 82.2 elaeostearate acid.
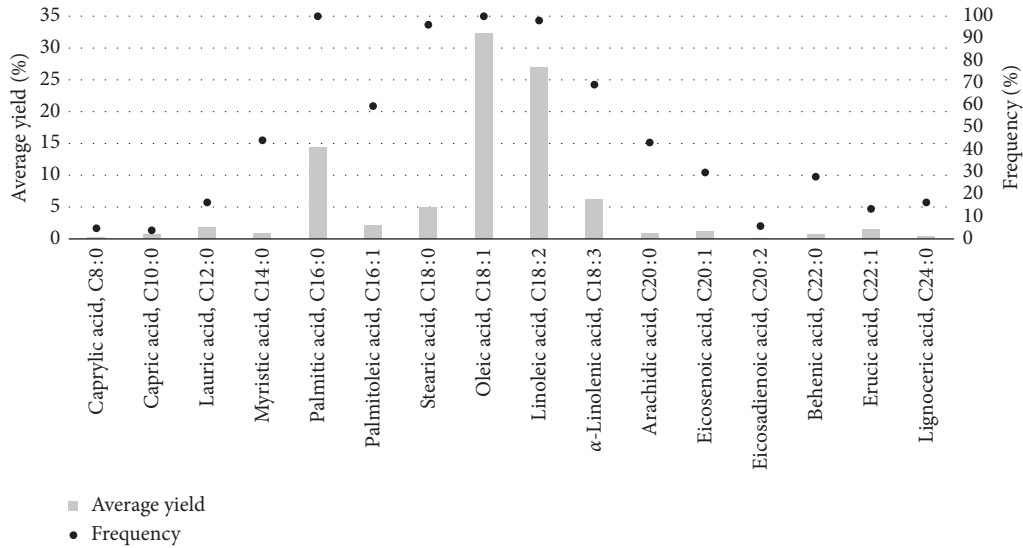
FIGURE 1: Percentage and frequency of each fatty oils in the biomasses reported in Table 1.
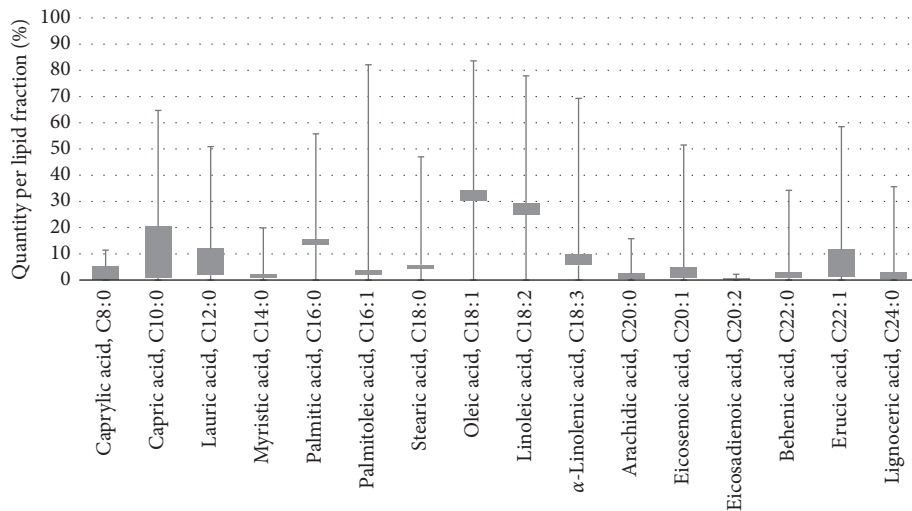

FIGURE 2: Average minimum and maximum (grey rectangle) and absolute maximum and minimum (interval lines).

While saturated acids are solid at room temperature, the unsaturated are in the liquid state. Furthermore, saturated and unsaturated fatty acids also differ regarding their structure. While saturated fatty acids have a linear molecule, the introduction of one or more double bonds promotes the molecule twisting and the possibility of geometrical isomerism. Figure 3 reports the difference in the structure for the fatty acid with 18 carbon atoms and 0, 1, and 2 double bonds.

Following the analysis summarized in Figures 1 and 2, the most common saturated and unsaturated fatty acids identified are presented in Table 2 together with the corresponding CAS number and their molecular weight.

4. Physical Properties

Temperature nondependent properties, namely, normal boiling point, normal melting point, critical properties, and acentric factor, were evaluated in this section.

Using the NIST database as a reference, the values obtained from the different estimation models and the values from the proposed correlations were compared using different deviation indexes:

(i) The absolute deviation (AD) is defined as

$$AD = |\text{estimated value} - \text{experimental value}|. \quad (1)$$

(ii) The relative deviation (RD) and the absolute relative deviation (ARD) are as follows, respectively:

$$RD = \frac{\text{estimated value} - \text{experimental value}}{\text{experimental value}} \times 100, \quad (2)$$

$$ARD = |RD|. \quad (3)$$

(iii) The average absolute deviation (AAD) is given as follows:

$$AAD = \frac{1}{n} \sum_{i=1}^{N} AD. \quad (4)$$

(a)   (b)   (c)
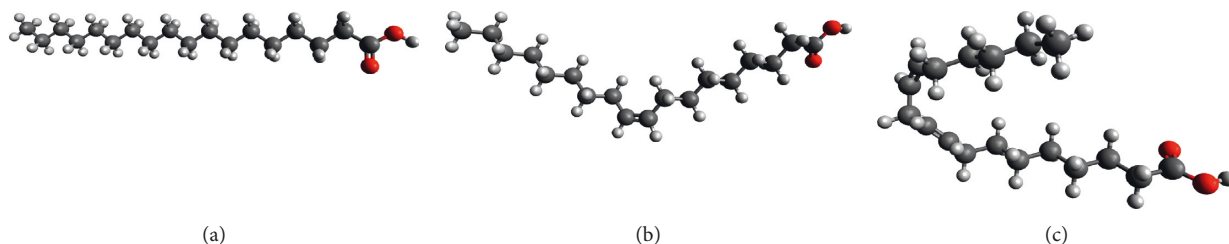
FIGURE 3: C18:0, stearic acid $C_{18}H_{36}O_2$ (a); C18:1, oleic acid $C_{18}H_{34}O_2$ (b); C18:2, linoleic acid $C_{18}H_{32}O_2$ (c).

TABLE 2: Fatty acids selected for the property evaluation classified by name, CAS number, and molecular weight.

CN:DB	Molecular formula	Common names and IUPAC name	CAS no.	MW (g/mol)
C8:0	$C_8H_{16}O_2$	Caprylic acid, n-octanoic acid	124-07-2	144.21
C10:0	$C_{10}H_{20}O_2$	Capric acid, n-decanoic acid	334-48-5	172.27
C12:0	$C_{12}H_{24}O_2$	Lauric acid, n-dodecanoic acid	143-07-7	200.32
C14:0	$C_{14}H_{28}O_2$	Myristic acid, tetradecanoic acid	544-63-8	228.38
C16:0	$C_{16}H_{32}O_2$	Palmitic acid, hexadecanoic acid	57-10-3	256.43
C18:0	$C_{18}H_{36}O_2$	Stearic acid, n-octadecanoic acid	57-11-4	284.48
C20:0	$C_{20}H_{40}O_2$	Arachidic acid, eicosanoic acid	506-30-9	312.54
C22:0	$C_{22}H_{44}O_2$	Behenic acid, docosanoic acid	112-85-6	340.59
C24:0	$C_{24}H_{48}O_2$	Lignoceric acid, tetracosanoic acid	557-59-5	368.65
C16:1	$C_{16}H_{30}O_2$	Palmitoleic acid, (9Z)-hexadec-9-enoic acid, cis-9-hexadecenoic acid	373-49-9	254.41
C18:1	$C_{18}H_{34}O_2$	Oleic acid, (9Z)-octadec-9-enoic acid, n-octadecenoic acid, [omega-9 fatty acid (18:1 ω9)]	112-80-1	282.47
C20:1	$C_{20}H_{38}O_2$	Paullinic acid, 13-eicosenoic acid, [omega-7 fatty acid (20:1 ω7)]	29204-02-2	310.52
		Gondoic acid, cis-gondoic acid, cis-11-eicosenoic acid, 11-eicosenoic acid, 11Z-eicosenoic acid, cis-11-icosenoic acid, (11Z)-icos-11-enoic acid, [omega-9 fatty acid (20:1 ω9)]	5561-99-9	
		Gadoleic acid, 9-eicosenoic acid, [omega-11 fatty acid (20:1 ω11)], (E)-icos-2-enoic acid	17735-94-3 26764-41-0	
C22:1	$C_{22}H_{42}O_2$	Erucic acid, (Z)-docos-13-enoic acid, cis-13-docosenoic acid	112-86-7	338.58
C24:1	$C_{24}H_{46}O_2$	Nervonic acid, (Z)-tetracos-15-enoic acid, [omega-9 fatty acid (24:1 ω9)]	506-37-6	366.62
C18:2	$C_{18}H_{32}O_2$	Linoleic acid, (9Z,12Z)-9,12-octadecadienoic acid, [omega-6 fatty acid (18:2 ω6)]	60-33-3	280.45
		α-Linolenic acid, cis-9,12,15-octadecatrienoic acid, [omega-3 fatty acid (18:2 ω3)]	463-40-1	
C18:3	$C_{18}H_{30}O_2$	Gamma-linolenic acid, gamolenic acid, all-cis-6,9,12-octadecatrienoic acid, [omega-6 fatty acid (18:2 ω6)]	506-26-3	278.44
		α-Calendic acid, (8E,10E,12Z)-octadeca-8,10,12-trienoic acid, [omega-6 fatty acid (18:2 ω6)]	5204-87-5	

(iv) The root mean square deviation or relative deviation (RMSD) is obtained using the following equation:

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N} AD^2}{N}}. \qquad (5)$$

(v) The average absolute relative deviation (AARD) is defined by the following equation:

$$\text{AARD} = \frac{1}{n}\sum_{i=1}^{N} \text{ARD}. \qquad (6)$$

4.1. Normal Boiling Point.
The normal boiling point (T_B) is defined as the temperature in which the vapor pressure equals the value of 1 atmosphere. The normal boiling point is used to

compare different liquids and represents an essential input for the estimation of other properties like the critical parameters.

4.1.1. Estimation Methods.
To determine the normal boiling point, several methods are available in the literature. The most relevant ones are summarized in Table 3.

Each of these methods has been applied for the set of fatty acids identified in Table 2.

The Joback and Reid method [148] estimates the normal boiling point considering the group incremental value (T_{B_i}) multiplied by the number of times the group appears in the compound (N_i). The estimation formula is reported in the following equation:

$$T_B = 198.2 + \sum_i N_i \cdot T_{b_i}. \qquad (7)$$

The coefficients used for the estimation of the normal boiling point are reported as Supplementary Material in Table A1.

Constantinou and Gani [149] established the two-level evaluation method reported as follows:

$$T_B(\text{K}) = 204.359 \cdot \ln\left(\sum_i N_i \cdot T_{b1i} + W \cdot \sum_j M_j \cdot T_{b2j}\right). \qquad (8)$$

The method is based on the first- and second-order group contribution. In the former, each group has a single contribution independently of the type of compound involved (T_{B1i}). The latter (T_{B2j}) has the function to provide more structural information about the portions of the structure where the description through the first-order groups is insufficient. The model constant W assumes the value zero if only the first-order group estimation is taken into account, or one if the second order is also considered. N_i and M_j are the group occurrences in the compound. The coefficients used to determine the normal boiling point are reported in Tables A2 and A3 of the Supplementary Material.

Marrero-Marejón and Pardillo-Fontdevila proposed a family of models to estimate the normal boiling point of pure organic compounds based on the compound chemical structure and molecular weight [150]. The normal boiling point is evaluated according to equation (9), where N_i is the number of times that type i occurs with contributions t_{bbk}:

$$T_B = \text{MW}^{-0.404} \sum_i N_i \cdot t_{bbk_i} + 156.0. \qquad (9)$$

In this case, the contributions are based on group interaction, taking into account the interactions between bonding groups in the molecule. Table A4, in the Supplementary Material, presents the coefficients used.

Marrero and Gani [151] defined an estimation of the normal boiling point based on three levels, as follows:

$$T_B(\text{K}) = 222.543 \cdot \ln\left(\sum_i N_i \cdot T_{b1i} + \sum_j M_j \cdot T_{b2j} + \sum_k O_j \cdot T_{b3k}\right). \qquad (10)$$

The first level includes the simple groups used for describing a wide variety of organic compounds. The second level involves groups that permit a better description of polyfunctional compounds and differentiation among isomers. Finally, the third level provides more structural information about molecular fragments of compounds whose description is insufficient through the first- and second-level groups. The coefficients to determine the normal boiling point can be found in Tables A5 and A6 of the Supplementary Material.

The estimation of the boiling point proposed by Nannoolal et al. [152] is reported as follows:

$$T_B(\text{K}) = \frac{\sum_i N_i C_i}{n^{0.6583} + 1.6868} + 84.3395, \qquad (11)$$

where C_i is the group contribution of group i and n is the number of atoms in the molecule (excluding the hydrogen atoms). The method is valid for nonelectrolyte organic compounds and was developed using experimental data for about 2850 compounds stored in the Dortmund data bank. Table A7 of the Supplementary Material presents the coefficients correspondent to this method.

4.1.2. Normal Boiling Point Estimation Results. The results for the normal boiling point estimated using the methods described are summarized in Table 4. The values extracted from the NIST database were accessed through the Aspen Property software, and they were used as a reference for the comparison with the estimated values. The values obtained were checked for consistency, and it was noticed that the normal boiling point for the C24:0 (673.7 K) was lower than the value reported for C22:0 (685.0 K). For this reason, the value of 704.4 K reported by Yaws [153] was used.

Figure 4 indicates the absolute relative deviation between the different methods when compared to the NIST values.

From Figure 4, it is possible to notice that the Joback and Raid method always overestimates the normal boiling point, and the overestimation increases with the molecular weight. In general, for the same number of atoms of carbon in the molecule, the overestimation increases with the unsaturation. The same trend, but with a reduced absolute relative deviation, is observed for the Marrero-Marejon and Pardillo-Fontdevila method. The opposite tendency is observed for the method developed by Constantinou and Gani, where the normal boiling point is underestimated for the saturated fatty acids with the highest molecular weight. A similar behaviour, but with a reduced margin of deviations, is observed for the Marrero and Gani method. The Nannoolal et al. method has a positive deviation for the unsaturated fatty acids that seem to be independent from the molecular weight. However, for unsaturated fatty acids, the overestimation increases with the molecular weight.

Table 5 shows the minimum and maximum absolute relative deviation for each method when compared with the data provided by the NIST database.

Among all the estimation methods explored, the two-level and the three-level approach proposed by Marrero and Gani provided a more reliable estimation of the normal boiling point for the FAs considered.

4.1.3. Novel Normal Boiling Point Estimation Method. Anand et al. [154] defined the normal boiling point for fatty acids methyl esters (FAMEs), as a function of molecular weight (equation (12)). The same approach was followed to propose an alternative correlation for the fatty acids:

$$T_{B_{\text{FAME}}} = A_{\text{FAME}}(\text{MW})^2 + B_{\text{FAME}}(\text{MW}) + C_{\text{FAME}}. \qquad (12)$$

Using a similar equation, it was possible to obtain the coefficients to determine the normal boiling points for the fatty acids considered by applying the generalized reduced gradient method to minimize the deviations. In fact,

TABLE 3: Methods for the normal boiling point estimation.

Method	Parameter(s) required
Joback and Reid [148]	Molecular structure
Constantinou and Gani [149]	Molecular structure
Marrero-Marejón and Pardillo-Fontdevila [150]	Molecular structure and MW
Marrero and Gani [151]	Molecular structure
Nannoolal et al. [152]	Molecular structure

TABLE 4: Comparison of experimental and estimated normal boiling temperature (K).

| CN : DB	NIST	Joback and Reid [148]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [152]
C8 : 0	512.6	528.2	512.2	518.2	517.8	516.1
C10 : 0	543.2	573.9	540.8	554.3	546.8	549.6
C12 : 0	572.1	619.7	565.9	588.3	572.5	580.0
C14 : 0	599.5	665.4	588.3	620.6	595.6	607.9
C16 : 0	619.8	711.2	608.5	651.4	616.4	633.7
C18 : 0	643.0	757.0	626.8	681.0	635.5	657.9
C20 : 0	672.9	802.7	643.7	709.5	653.1	680.6
C22 : 0	692.9	848.5	659.2	737.1	669.4	702.1
C24 : 0	704.4*	894.2	673.7	763.8	684.5	722.4
C16 : 1	632.5	715.4	607.0	653.4	617.5	625.8
C18 : 1	635.9	761.1	625.5	682.9	636.5	650.4
C20 : 1	642.4	806.9	642.4	711.4	654.0	673.5
C22 : 1	665.7	852.6	658.1	738.8	670.2	695.3
C24 : 1	672.6	898.4	672.6	765.5	685.3	715.9
C18 : 2	624.1	765.3	624.1	684.8	637.5	643.0
C18 : 3	622.7	769.4	622.7	686.7	638.5	635.5

*Value reported by Yaws [153].
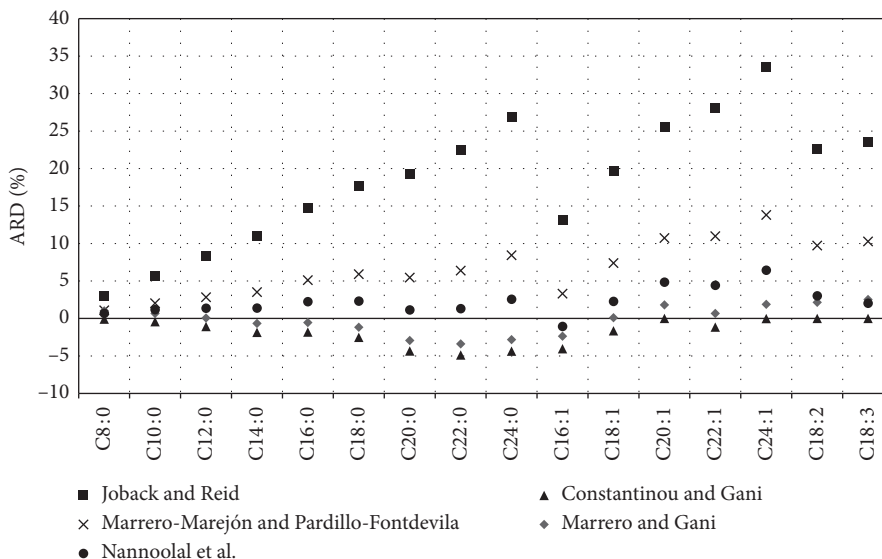
FIGURE 4: Absolute relative deviation comparison for the normal boiling point estimation.

observing the normal boiling point values, as a function of the molecular weight, it is possible to conclude that it has a parabolic behaviour.

The novel estimation method, reported in equation (13), has three coefficients, assigned as $A_{T_{B_{\text{FA}}\text{CN}:n}}$, $B_{T_{B_{\text{FA}}\text{CN}:n}}$, and $C_{T_{B_{\text{FA}}\text{CN}:n}}$, and a correction factor, $\alpha_{T_B\text{CN}:n}$, which depends on the number of unsaturation:

$$T_{B_{\text{FA}}} = \alpha_{T_B\text{CN}:n} \cdot \left[A_{A_{T_{B_{\text{FA}}\text{CN}:n}}} (\text{MW})^2 + B_{T_{B_{\text{FA}}\text{CN}:n}} (\text{MW}) + C_{T_{B_{\text{FA}}\text{CN}:n}} \right]. \tag{13}$$

The values for $A_{T_{B_{\text{FA}}\text{CN}:n}}$, $B_{T_{B_{\text{FA}}\text{CN}:n}}$ $C_{T_{B_{\text{FA}}\text{CN}:n}}$, and $\alpha_{T_B\text{CN}:n}$ were obtained by minimizing the relative deviations with the

TABLE 5: Deviations of the different methods for the normal boiling point estimation.

	Joback and Reid [148]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [152]
AAD (K)	119.60	11.55	43.23	10.05	15.43
RMSD (K)	133.05	16.40	49.56	12.33	18.65
AARD (%)	18.5	1.8	6.7	1.6	2.4
MIN RD (%)	3	−5	1	−3	−11
MAX RD (%)	34	0	14	3	6

NIST database values, using the GRG nonlinear solving method to achieve the optimized result. The coefficients obtained are presented in Table 6.

The proposed normal boiling point estimation method showed a lower estimation deviation when compared with the other methods previously presented. In particular, it was obtained: AAD = 8.49 K, RMSD = 11.94 K, AARD = 1.3%, MIN RD = −3.6%, and MAX RD = 4.3%.

4.2. Normal Melting Point.
The normal melting point for a pure substance is defined as the temperature in which the solid and the liquid form exist in equilibrium at atmospheric pressure. In general, it is expected that the melting point of fatty acids increases if the unsaturation is reduced. If the fatty acids are used for biodiesel production, the availability of the melting point is essential for the evaluation of the cold-flow properties.

4.2.1. Estimation Methods.
Several methods are available in the literature to determine the normal melting point. The most appropriate methods are gathered in Table 7.

Joback and Reid proposed the estimation formula reported as follows [148]:

$$T_M\,(\text{K}) = 122.5 + \sum N_i \cdot T_{m_i}. \tag{14}$$

According to the authors, however, estimations of the normal melting point are not accurate and should be considered only as approximate. The coefficients of the group contributions are presented in Table A1 of the Supplementary Material.

The Constantinou and Gani method [149] is presented as follows:

$$T_M\,(\text{K}) = 102.425 \times \ln\!\left(\sum_i N_i \times T_{m1i} + W \times \sum_j M_j \times T_{m2j} \right). \tag{15}$$

The coefficients to determine the normal melting point can be found in Tables A2 and A3 of the Supplementary Material.

Marrero and Gani [151] developed a method to determine the normal melting point using the following equation:

$$T_M\,(\text{K}) = 147.450 \times \ln\!\left(\sum_i N_i \times T_{m1i} + \sum_j M_j \times T_{m2j} \right.$$
$$\left. + \sum_k O_j \times T_{m3k} \right). \tag{16}$$

TABLE 6: Coefficients for the estimation of the normal boiling point according to equation (13).

Coefficients	Values
$A_{T_{B_{\text{FA CN}:n}}}$	$-7.0670E-04$
$B_{T_{B_{\text{FA CN}:n}}}$	0.9173
$C_{T_{B_{\text{FA CN}:n}}}$	205.6120
$\alpha_{T_B\text{CN}:0}$	1.5697
$\alpha_{T_B\text{CN}:1}$	1.5501
$\alpha_{T_B\text{CN}:2}$	1.5323
$\alpha_{T_B\text{CN}:3}$	1.5329

TABLE 7: Methods for the normal melting point estimation.

Method	Parameter required
Joback and Reid [148]	Molecular structure
Constantinou and Gani [149]	Molecular structure
Marrero and Gani [151]	Molecular structure

The coefficients to determine the normal melting point can be found in Tables A5 and A6 of the Supplementary Material.

4.2.2. Normal Melting Point Estimation Results.
Table 8 presents the values of the estimated normal melting point together with the values obtained from the NIST database.

Figure 5 reports the absolute relative deviation between the different methods when compared with the NIST values.

The Joback and Reid group contribution method overestimates the normal melting point. The overestimation regularly grows for saturated fatty acids with a consistent penalty for molecules with the highest molecular weight. The same trend is observed for the unsaturated compounds even if the increase of the absolute relative deviation is lower with respect to the case of saturated fatty acids.

Table 9 shows the deviation indexes for each method when compared with the data provided by NIST.

The method of Constantinou and Gani offers the best estimation with a very good prediction of the saturated compounds. However, for the unsaturated fatty acids, all the methods considered report a high estimation deviation. When comparing molecules with the same number of carbons, it is possible to observe that the melting point decreases when the unsaturation increases. This decrease is due to the molecular distortion induced by the double bonds that prevent the molecules from packing together easily. The difficulty in predicting the London dispersion forces between the oil molecules may be the cause of the high deviations observed for unsaturated fatty acids.

TABLE 8: Comparison of experimental and estimated normal melting point (K).

CN : DB	NIST	Joback and Reid [148]	Constantinou and Gani [149]	Marrero and Gani [151]
C8 : 0	289.7	340.5	293.6	333.6
C10 : 0	304.5	363.1	303.8	341.2
C12 : 0	317.0	385.6	313.2	348.3
C14 : 0	327.3	408.1	321.7	355.1
C16 : 0	335.6	430.7	329.6	361.7
C18 : 0	342.6	453.2	336.9	367.9
C20 : 0	348.2	475.8	343.7	373.9
C22 : 0	353.8	498.3	350.1	379.7
C24 : 0	355.6	520.8	356.1	385.2
C16 : 1	274.8	425.6	326.2	365.9
C18 : 1	286.5	448.1	333.8	371.9
C20 : 1	297.3	470.7	340.8	377.8
C22 : 1	306.1	493.2	347.4	383.4
C24 : 1	—	515.8	353.6	388.8
C18 : 2	267.6	443.1	330.6	375.8
C18 : 3	260.0	438.0	327.2	379.7
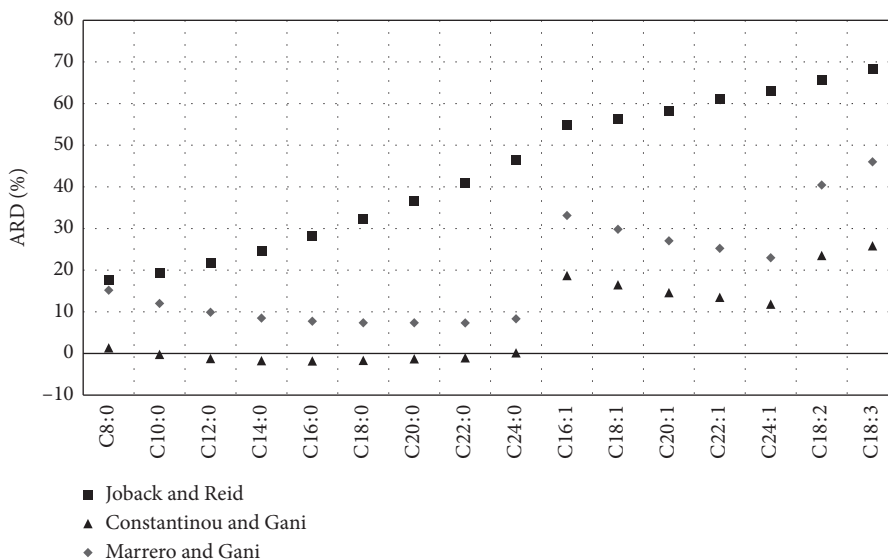
FIGURE 5: Absolute relative deviation comparison for the normal melting point estimation.

TABLE 9: Deviations of different methods for the estimation of the normal melting point.

	Joback and Reid [148]	Constantinou and Gani [149]	Marrero and Gani [151]
AAD (K)	132.98	24.10	56.68
RMSD (K)	141.25	34.02	65.14
AARD (%)	43.5	8.4	19.3
MIN RD (%)	18	−2	7
MAX RD (%)	69	26	46

4.2.3. Novel Normal Melting Point Estimation Method.

It is possible to obtain the coefficients to determine the normal melting points applying the generalizedreduced gradient (GRG) method to minimize the deviations, with a similar procedure described in Section 4.1.3 for the estimation of the normal boiling point.

Equation (17) is the novel estimation method developed:

$$T_{M_{\text{FA}}} = \alpha_{T_M \text{CN:}n} \cdot \left[A_{T_{M_{\text{FA}}}} (\text{MW})^2 + B_{T_{M_{\text{FA}}}} (\text{MW}) + C_{T_{M_{\text{FA}}}} \right]. \tag{17}$$

The main advantage of this method is the possibility of estimating the normal meting point, using the fatty acids' molecular weight exclusively.

The coefficients $A_{T_{M_{\text{FA CN:}n}}}$, $B_{T_{M_{\text{FA CN:}n}}}$, $C_{T_{B_{\text{FA CN:}n}}}$, and $\alpha_{T_M \text{CN:}n}$ were obtained by minimizing the relative deviations with the NIST database values. The obtained coefficients are presented in Table 10.

For the proposed method, the comparison indexes are AAD = 3.15 K, RMSD = 4.09 K, AARD = 1.0%, MIN RD = −2.6%, and MAX RD = 3.1%, giving a smaller deviation when compared to the other estimation methods.

4.3. Critical Parameters. The critical point is used to identify the fluid region where the liquid and gas phases can be no longer distinguished. Critical parameters are used for the estimation of other properties, such as the acentric factor, compressibility factor, liquid density, vapor pressure, and enthalpy of vaporization, among others.

4.3.1. Estimation Methods. Several methods are available in the literature to determine the critical parameters such as critical temperature, critical pressure, and critical volume. The most appropriate methods are summarized in Table 11.

Joback and Reid proposed the relations reported in equations (18)–(20) to estimate the critical properties based on the group contribution methods [148]:

$$T_C = \frac{T_B}{0.584 + 0.965 \sum N_i \cdot T_{c_i} - \left(\sum N_i \cdot T_{c_i}\right)^2}, \tag{18}$$

$$P_C = \frac{1}{\left(0.113 + 0.0032 N_A - \sum N_i \cdot P_{c_i}\right)^2}, \tag{19}$$

$$V_C = 17.5 + \sum N_i \cdot V_{c_i}, \tag{20}$$

where N_A is the number of atoms in the molecule. The values T_{c_i}, P_{c_i}, and V_{c_i} are presented in Table A1.

Constantinou and Gani [149] established a method to determine T_C, P_C, and V_C using equations (21)–(23), respectively:

$$T_C \text{ (K)} = \frac{T_B}{\left(0.048271 - 0.019846 N_r + \sum_k N_k \cdot t_{ck} + \sum_j M_j \Delta t_{cj}\right)^{0.2}}, \tag{24}$$

$$P_C \text{ (bar)} = \frac{0.0186233 \cdot T_C}{-0.96601 + \exp\left(-0.0092295 - 0.0290403 N_r + 0.041\left(\sum_k N_k \cdot P_{cbk} + \sum_j M_j \Delta P_{cj}\right)\right)}. \tag{25}$$

The coefficients to determine these critical properties can be found in Table A6 in the Supplementary Material.

Marrero-Marejón and Pardillo-Fontdevila developed equations (26)–(28) to calculate the critical parameters [150]:

$$T_C \text{ (K)} = \frac{T_B}{0.5851 - 0.9286\left(\sum_k N_k \cdot t_{bck}\right) + \left(\sum_j M_j \cdot \Delta t_{cbj}\right)^2}, \tag{26}$$

$$P_C \text{ (bar)} = \left(0.1285 - 0.0059 N_{\text{atoms}} - \sum_k N_k \cdot P_{cbk}\right)^{-2}, \tag{27}$$

$$V_C \left(\text{cm}^3 \cdot \text{mol}^{-1}\right) = -25.1 + \sum_k N_k \cdot v_{cbk}, \tag{28}$$

where N_{atoms} is the number of atoms in the compound and N_k is the number of atoms of type k with contributions t_{cbk}, p_{cbk},

TABLE 10: Coefficients for the estimation of the normal melting point according to equation (17).

Coefficients	Values
$A_{T_{M_{\text{FACN}:n}}}$	$-4.1905E-04$
$B_{T_{M_{\text{FACN}:n}}}$	0.4863
$C_{T_{M_{\text{FACN}:n}}}$	193.9418
$\alpha_{T_M \text{CN}:0}$	1.1380
$\alpha_{T_M \text{CN}:1}$	0.9752
$\alpha_{T_M \text{CN}:2}$	0.8999
$\alpha_{T_M \text{CN}:3}$	0.8759

$$T_C \text{ (K)} = 181.128 \cdot \ln\left(\sum_i N_i \cdot T_{c1i} + W \cdot \sum_j M_j \cdot T_{c2j}\right), \tag{21}$$

$$P_C \text{ (bar)} = \left(\sum_i N_i \cdot P_{c1i} + W \times \sum_j M_j \cdot P_{c2j} + 0.100220\right)^{-2} + 1.3705, \tag{22}$$

$$V_C \left(\text{cm}^3 \cdot \text{mol}^{-1}\right) = -0.004350 + \left(\sum_i N_i \cdot v_{c1i} + W \times \sum_j M_j \cdot v_{c2j}\right). \tag{23}$$

The coefficients to determine the critical properties can be found in Tables A2 and A3 in the Supplementary Material.

Wilson and Jasperson suggested equation (24) to estimate the critical temperature and equation (25) to determine the critical pressure:

and v_{cbk}. The parameters to determine these critical parameters can be found at Table A4 in the Supplementary Material.

Marrero and Gani [151] determined T_C, P_C, and V_C using the following equations:

$$T_C \text{ (K)} = 231.239 \cdot \ln\left(\sum_i N_i \cdot T_{c1i} + W \cdot \sum_j M_j \cdot T_{c2j} + W \cdot \sum_k O_k \cdot T_{c3k}\right), \tag{29}$$

$$P_C \text{ (bar)} = \left(\sum_i N_i \cdot P_{c1i} + W \times \sum_j M_j \cdot P_{c2j} + W \times \sum_k O_k \cdot P_{c3k} + 0.108998\right)^{-2} + 5.9827, \tag{30}$$

TABLE 11: Methods for the critical parameters' estimation.

Method	Parameter(s) required
Joback and Reid [148]	Molecular structure and T_B
Constantinou and Gani [149]	Molecular structure
Wilson and Jasperson [155]	Molecular structure and T_B
Marrero-Marejón and Pardillo-Fontdevila [150]	Molecular structure and T_B
Marrero and Gani [151]	Molecular structure
Nannoolal et al. [156]	Molecular structure, MW, and T_B

$$V_C \left(\text{cm}^3 \cdot \text{mol}^{-1}\right) = 7.95 + \left(\sum_i N_i \cdot V_{c1i} + W \times \sum_j M_j \cdot V_{c2j} \right.$$
$$\left. + W \times \sum_k O_k \cdot V_{c3k} \right). \tag{31}$$

The coefficients to determine the critical properties can be found in Tables A5 and A6 in the Supplementary Material.

The estimation of the critical properties proposed by Nannoolal et al. [156] is presented in the following equations:

$$T_C \ (\text{K}) = T_B \left(0.6990 + \frac{1}{0.9889 + \left(\sum_i N_i C_i\right)^{0.8607}} \right), \tag{32}$$

$$P_C \ (\text{kPa}) = \frac{\text{MW}^{-0.14041} \ (\text{g/mol})}{\left(0.00939 + \sum_i N_i C_i\right)^2}, \tag{33}$$

$$V_C \left(\text{cm}^3 \cdot \text{mol}^{-1}\right) = \frac{\sum_i N_i C_i}{n^{-0.2266}} + 86.1539, \tag{34}$$

where n is the number of atoms in the molecule (excluding hydrogen). Table A7 in the Supplementary Material presents the coefficients used.

For the estimation methods that depend on the normal boiling point temperature, this value can be experimentally determined or estimated. The calculations were performed using the normal boiling point temperatures available from the NIST database, as reported in Table 4.

4.3.2. Critical Properties Estimation Results

(1) Critical Temperature Estimation Results. The estimated and experimental values for the critical temperatures are presented in Table 12.

Figure 6 presents the absolute relative deviation between the methods considered and the NIST database values.

Except for the Marrero and Gani's method, all the other methods have a general agreement until the C16 : 0. For the compounds with higher molecular weight, the method developed by Nannoolal et al. and by Constantinou and Gani

give the best results. When one or more unsaturations are considered, it is not possible to define a method that consistently predicts the critical temperature. Table 13 shows the minimum and maximum absolute relative deviation for each method when compared with the data provided by NIST.

From the analysis of Table 13, it is possible to notice that the Constantinou and Gani's method exhibits the best global performances for the critical temperature estimation.

(2) Critical Pressure Estimation Results. The results for the estimated critical pressures and the experimental values for the fatty acids are presented in Table 14.

Figure 7 presents the relative deviation between the estimated values and the ones gathered from the NIST database. All the methods provide estimations included in a range of deviation of ±10%, except for the Marrero and Gani method when applied to saturated fatty acids with high molecular weight and unsaturated fatty acids with one and three double bonds. The Nannoolal et al. method gives the best estimation for the fatty acids at high molecular weight with one double bond. Regarding the saturated compounds, the Marrero-Marejón and Pardillo-Fontdevila method overestimates the critical pressure until C16 : 0. After this component, there is an underestimation that increases linearly with the molecular weight. Apart from the Marrero and Gani method, all the others underestimate the critical pressure in the range of C16 : 0–C22 : 0.

Table 15 shows the minimum and maximum absolute relative deviation for each method when compared with the data provided by NIST.

(3) Critical Volume Estimation Results. The estimated and experimental values for the fatty acids' critical volume are presented in Table 16.

Figure 8 presents the relative deviation distribution between the estimated values and the ones provided by NIST.

The Nannoolal et al. method offers the best prediction for the saturated compounds with a peak of about 10% overestimation for C24 : 0. However, the overestimation increases to 20% when the unsaturated compounds are evaluated. All the other methods exhibit an opposite behaviour, with the tendency to underestimate the critical

TABLE 12: Comparison of experimental and estimated critical temperature (K).

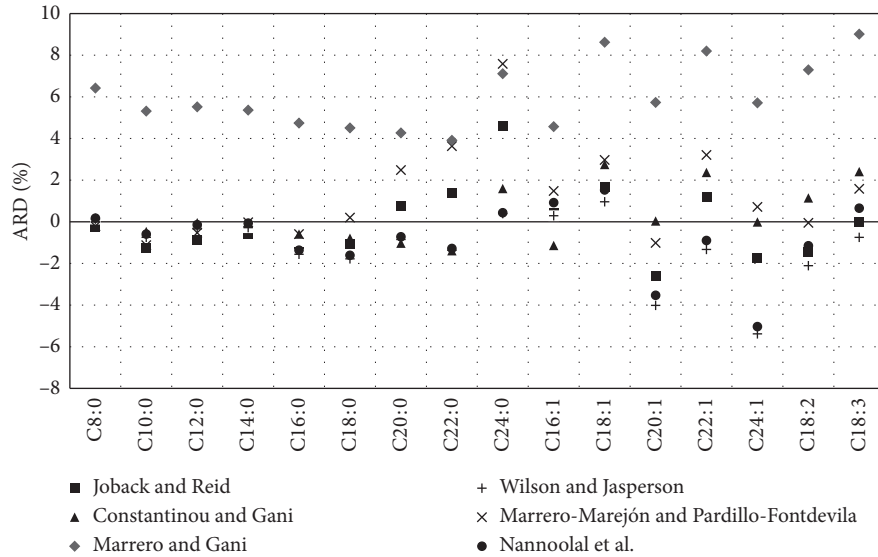| CN : DB	NIST	Joback and Reid [148]	Wilson and Jasperson [155]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [156]
C8 : 0	693.7	692.1	694.6	695.0	692.3	738.2	694.9
C10 : 0	723.8	714.6	718.4	720.4	715.7	762.3	719.5
C12 : 0	743.0	736.6	740.5	742.7	739.1	784.0	742.0
C14 : 0	763.0	758.4	760.8	762.5	762.8	803.9	762.5
C16 : 0	785.0	773.5	772.7	780.4	780.4	822.2	774.3
C18 : 0	803.0	794.5	788.7	796.6	804.6	839.2	790.1
C20 : 0	820.0	826.2	813.0	811.6	840.4	855.0	814.1
C22 : 0	837.0	848.4	825.5	825.4	867.4	869.8	826.3
C24 : 0	825.0	863.1	828.2	838.2	887.6	883.7	828.6
C16 : 1	789.0	792.5	791.3	780.0	800.7	825.1	796.3
C18 : 1	775.0	787.9	782.4	796.3	798.1	841.8	786.9
C20 : 1	811.0	790.1	778.4	811.3	802.8	857.5	782.4
C22 : 1	806.0	815.6	795.3	825.1	831.9	872.1	798.8
C24 : 1	838.0	823.7	792.9	837.9	844.0	885.9	795.8
C18 : 2	787.0	775.8	770.4	796.0	786.6	844.5	778.0
C18 : 3	777.0	776.8	771.2	795.7	789.3	847.1	782.1

FIGURE 6: Absolute relative deviation of estimation for the critical temperature.

TABLE 13: Deviations of different methods for the estimation of the critical temperature.

	Joback and Reid [148]	Wilson and Jasperson [155]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [156]
AAD (K)	10.64	11.23	7.95	13.80	47.23	10.14
RMSD (K)	13.72	16.13	10.57	20.85	48.77	14.62
AARD (%)	1.3	1.4	1.0	1.7	6.0	1.3
MIN RD (%)	−3	−5	−1	−1	4	−5
MAX RD (%)	2	1	3	4	9	2

volume for saturated compounds, with a lower deviation for the unsaturated fatty acids.

Table 17 shows the minimum and maximum absolute relative deviation for each method when compared with the data provided by the NIST database.

Except for the Nannoolal et al. method, that is only recommended for saturated compounds, all the other methods provide a general agreement in the critical volume estimation.

4.3.3. Novel Critical Parameters Estimation Method

(1) Novel Critical Temperature Estimation Method. Anand et al. [154] proposed a critical temperature estimation method for FAMEs, according to the following:

$$T_{C_{FAME}} = A_{T_{C_{FAME}}} (MW)^2 + B_{T_{C_{FAME}}} (MW) + C_{T_{C_{FAME}}}. \quad (35)$$

TABLE 14: Comparison of experimental and estimated critical pressure (bar).

CN : DB	NIST	Joback and Reid [148]	Wilson and Jasperson [155]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [156]
C8 : 0	28.57	27.79	26.91	27.67	31.07	26.87	26.27
C10 : 0	20.76	22.92	22.22	22.79	25.40	22.52	22.11
C12 : 0	19.31	19.22	18.79	19.14	21.16	19.40	18.87
C14 : 0	16.40	16.35	16.17	16.36	17.89	17.09	16.29
C16 : 0	14.90	14.08	13.96	14.18	15.33	15.33	14.21
C18 : 0	13.30	12.25	12.25	12.44	13.28	13.95	12.50
C20 : 0	12.00	10.76	10.97	11.03	11.62	12.86	11.07
C22 : 0	11.10	9.52	9.75	9.88	10.25	11.98	9.88
C24 : 0	8.49	8.49	8.61	8.92	9.11	11.25	8.86
C16 : 1	14.88	14.65	14.58	14.15	15.86	15.52	14.37
C18 : 1	13.90*	12.71	12.39	12.42	13.71	14.10	12.63
C20 : 1	10.98	11.13	10.69	11.02	11.96	12.98	11.18
C22 : 1	9.83	9.83	9.55	9.87	10.53	12.07	9.97
C24 : 1	8.87	8.75	8.61	8.91	9.35	11.33	8.94
C18 : 2	14.10	13.19	12.43	12.40	14.15	14.25	12.76
C18 : 3	12.34*	13.71	12.68	12.38	14.62	14.41	12.89

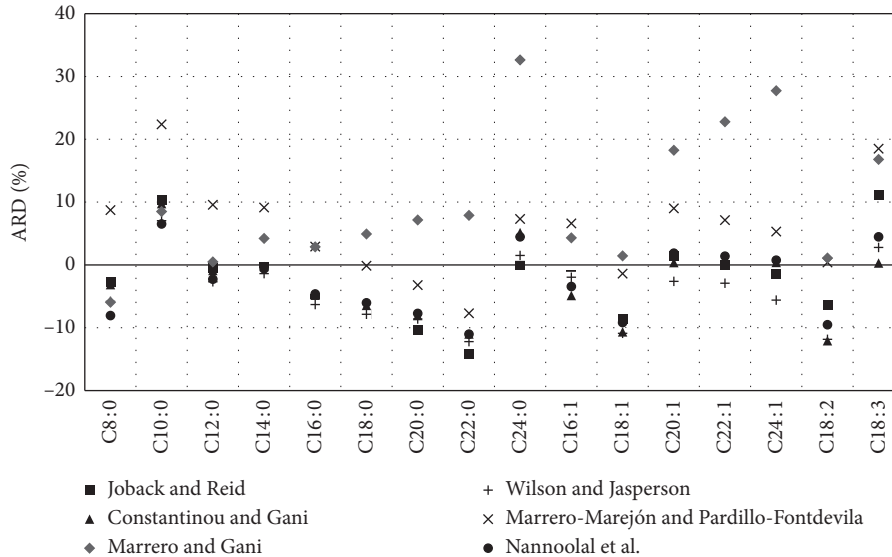*Values retrieved from the database APV88 PURE32 of Aspen Plus.

FIGURE 7: Absolute relative deviation of estimation for the critical pressure.

TABLE 15: Deviations of different methods for the estimation of the critical pressure.

NIST	Joback and Reid [148]	Wilson and Jasperson [155]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [156]
AAD (bar)	0.73	0.83	0.71	1.15	1.23	0.77
RMSD (bar)	0.98	0.99	0.95	1.64	1.50	0.97
AARD (%)	5.1	5.7	4.9	7.5	10.4	5.1
MIN RD (%)	−14	−12	−12	−8	−6	−11
MAX RD (%)	11	7	10	22	33	7

Globally, the Nannoolal et al. method offers a better estimation together with the Constantinou and Gani approach.

Using a similar equation, it is possible to obtain the coefficients to determine the critical temperature for the fatty acids applying the generalized reduced gradients method to minimize the deviations. Equation (36) is the novel estimation method proposed to estimate the fatty acids critical temperature:

$$T_{C_{FA}} (K) = \alpha_{T_C CN:n} \cdot \left[A_{T_{C_{FA}}} (MW)^2 + B_{T_{C_{FA}}} (MW) + C_{T_{C_{FA}}} \right]. \tag{36}$$

The coefficients $A_{T_{C_{FA} CN:n}}$, $B_{T_{C_{FA} CN:n}}$, $C_{T_{C_{FA} CN:n}}$, and $\alpha_{T_C CN:n}$ were obtained by minimizing the relative deviations with the

TABLE 16: Comparison of experimental and estimated critical volume (m³/kmol).

CN : DB	NIST	Joback and Reid [148]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [156]
C8:0	0.526	0.5075	0.5071	0.5107	0.5046	0.5267
C10:0	0.639	0.6195	0.6187	0.6239	0.6172	0.6579
C12:0	0.787	0.7315	0.7302	0.7371	0.7298	0.7948
C14:0	0.921	0.8435	0.8417	0.8503	0.8423	0.9367
C16:0	1.066	0.9555	0.9532	0.9635	0.9549	1.0831
C18:0	1.255	1.0675	1.0647	1.0767	1.0674	1.2335
C20:0	1.371	1.1795	1.1763	1.1899	1.1800	1.3877
C22:0	1.486	1.2915	1.2878	1.3031	1.2926	1.5453
C24:0	1.575	1.4035	1.3993	1.4163	1.4051	1.7062
C16:1	0.898	0.9355	0.9399	0.9429	0.9409	1.0525
C18:1	1.016	1.0475	1.0514	1.0561	1.0535	1.2022
C20:1	1.158	1.1595	1.1630	1.1693	1.1660	1.3557
C22:1	1.448	1.2715	1.2745	1.2825	1.2786	1.5127
C24:1	1.402	1.3835	1.3860	1.3957	1.3911	1.6729
C18:2	0.972	1.0275	1.0381	1.0355	1.0395	1.1708
C18:3	0.960	1.0075	1.0248	1.0149	1.0255	1.1395
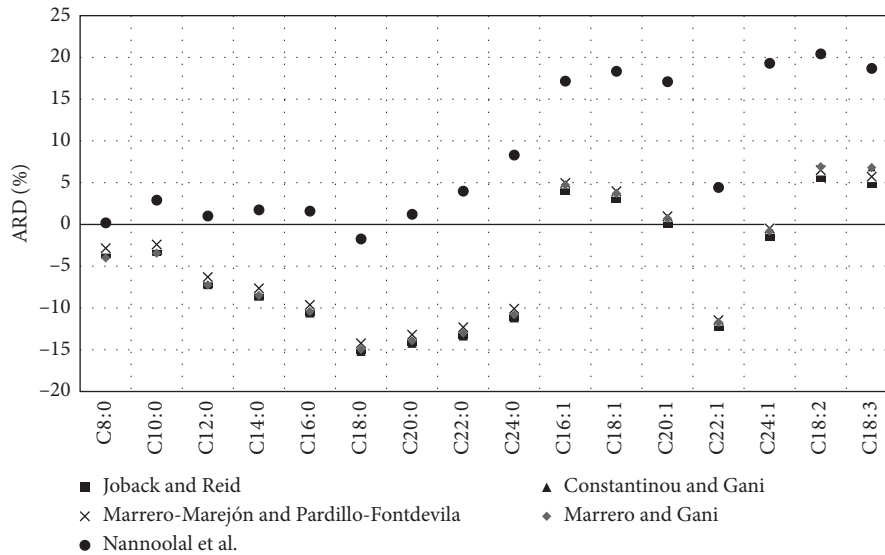
FIGURE 8: Absolute relative deviations of estimation for the critical volume.

NIST database values. The coefficients obtained are presented in Table 18.

For the proposed method, the critical temperature deviations resulted in AAD = 5.88 K, RMSD = 8.01 K, AARD = 0.7%, MIN RD = −1.6%, and MAX RD = 2.3% compared with NIST database. Thus, AAD, RMSD, and AARD significantly outperform the estimation methods considered.

(2) Novel Critical Pressure Evaluation Method. Applying the same procedure, it is possible to optimize equation (37) in order to obtain a functional equation to estimate the critical pressure:

$$P_{C_{FA}}(\text{bar}) = \alpha_{P_C \text{CN}:n} \cdot \left[A_{P_{C_{FA}}}(\text{MW})^2 + B_{P_{C_{FA}}}(\text{MW}) + C_{P_{C_{FA}}} \right]. \tag{37}$$

The coefficients $A_{P_{C_{FA} \text{CN}:n}}$, $B_{P_{C_{FA} \text{CN}:n}}$, $C_{P_{C_{FA} \text{CN}:n}}$, and $\alpha_{P_C \text{CN}:n}$ were obtained by minimizing the relative deviations with the

NIST database values, using the GRG nonlinear solving method to find the optimized result. The obtained coefficients are presented in Table 19.

For the proposed method, the critical pressure deviations resulted in AAD = 0.69 bar, RMSD = 0.94 bar, AARD = 4.6%, MIN RD = −10.4%, and MAX RD = 9.7%. Again, AAD, RMSD, and AARD show an improvement in accuracy, when compared with the considered estimation methods.

(3) Novel Critical Volume Estimation Method. Applying the same procedure as it was suggested before, it is possible to derive equation (38) to estimate the critical volume:

$$V_{C_{FA}}(\text{mL/mol}) = \alpha_{V_C \text{CN}:n} \cdot \left[A_{V_{C_{FA}}}(\text{MW})^2 + B_{V_{C_{FA}}}(\text{MW}) + C_{V_{C_{FA}}} \right]. \tag{38}$$

The coefficients $A_{V_{C_{FA} \text{CN}:n}}$, $B_{V_{C_{FA} \text{CN}:n}}$, $C_{V_{C_{FA} \text{CN}:n}}$, and $\alpha_{V_C \text{CN}:n}$ were obtained by minimizing the relative deviations with the

TABLE 17: Deviations of different methods for the estimation of the critical volume.

	Joback and Reid [148]	Constantinou and Gani [149]	Marrero-Marejón and Pardillo-Fontdevila [150]	Marrero and Gani [151]	Nannoolal et al. [156]
AAD (m^3/kmol)	0.087	0.091	0.084	0.090	0.096
RMSD (m^3/kmol)	0.112	0.114	0.106	0.112	0.130
AARD (%)	7.3	7.6	7.0	7.6	8.6
MIN RD (%)	−5	−15	−15	−14	−15
MAX RD (%)	31	6	7	7	7

TABLE 18: Coefficients for the estimation of the critical temperature according to equation (36).

Coefficients	Values
$A_{T_{C_{FA\,CN:n}}}$	$-1.8345E-03$
$B_{T_{C_{FA\,CN:n}}}$	1.6239
$C_{T_{C_{FA\,CN:n}}}$	550.5882
$\alpha_{T_C CN:0}$	0.9286
$\alpha_{T_C CN:1}$	0.9185
$\alpha_{T_C CN:2}$	0.9134
$\alpha_{T_C CN:3}$	0.9028

TABLE 19: Coefficients for the estimation of the critical pressure according to equation (37).

Coefficients	Values
$A_{P_{C_{FA\,CN:n}}}$	$7.0357E-04$
$B_{P_{C_{FA\,CN:n}}}$	-0.5776
$C_{P_{C_{FA\,CN:n}}}$	143.4049
$\alpha_{P_C CN:0}$	0.3515
$\alpha_{P_C CN:1}$	0.3556
$\alpha_{P_C CN:2}$	0.3836
$\alpha_{P_C CN:3}$	0.3323

NIST database values, using the GRG nonlinear solving method to achieve the optimized result. The obtained coefficients are presented in Table 20.

The proposed method for the critical volume yield deviations of AAD = 0.03 (m^3/kmol), RMSD = 0.05 (m^3/kmol), AARD = 2.1%, MIN RD = −13.6%, and MAX RD = 3.1%. The first three indicators significantly outperform the ones computed for the considered estimation methods.

4.4. Acentric Factor.

The acentric factor (ω) is a pure component constant that indicates the acentricity or nonsphericity of a molecule. Monoatomic molecules are expected to have acentric factors equal to zero, and their values increase with the molecular weight and polarity [155].

This property is used in the estimation of transport and thermodynamic properties for gases and liquids, such as compressibility factor, heat capacity, enthalpy of vaporization, and saturated density [155, 157].

4.4.1. Estimation Method.

Several methods are available in the literature to determine the acentric factor. The most appropriate methods are summarized in Table 21.

The acentric factor was initially proposed by Pitzer et al., and it is given by the following equation [158]:

$$\omega = -\log_{10} P_r - 1.0, \tag{39}$$

TABLE 20: Coefficients for the estimation of the critical volume according to equation (38).

Coefficients	Values
$A_{V_{C_{FA\,CN:n}}}$	$-1.0023E-06$
$B_{V_{C_{FA\,CN:n}}}$	0.0206
$C_{V_{C_{FA\,CN:n}}}$	-0.9068
$\alpha_{V_C CN:0}$	0.2485
$\alpha_{V_C CN:1}$	0.2106
$\alpha_{V_C CN:2}$	0.2033
$\alpha_{V_C CN:3}$	0.2025

TABLE 21: Methods for the estimation of the acentric factor.

Method	Parameters required
Pitzer et al. [158]	Vapor pressure and P_C
Lee and Kesler [159]	T_B, T_C, P_C
Watanasiri et al. [160]	Specific gravity, MW, T_B
Ambrose and Walton [161]	T_B, T_C, P_C
Chen et al. [157]	T_B, T_C, P_C
Constantinou et al. [162]	Molecular structure

where P_r is the reduced vapor pressure, defined as $P_r = P^{vap}/P_C$, and P^{vap} is the vapor pressure at temperature T, defined at the reduced temperature $T/T_C = 0.7$. The vapor pressure can be determined by the NIST Wagner Equation, given as follows:

$$\ln\left(P^{vap}\right) = C_5 + \frac{C_1 \times \left(1 - (T/C_6)\right) + C_2 \times \left(1 - (T/C_6)\right)^{1.5} + C_3 \times \left(1 - (T/C_6)\right)^{2.5} + C_4 \times \left(1 - (T/C_6)\right)^{5}}{T/C_6}, \tag{40}$$

where the pressure is given in Pa. The coefficients C_1, C_2, C_3, C_4, C_5, and C_6 can be found in Table A7 of the Supplementary Material.

The parameter proposed by Pitzer et al. is, however, limited to reduced temperatures above 0.8.

Lee and Kesler proposed an analytical correlation for the acentric factor employing equations of state, based on a wide variety of compounds. Their goal was to improve the representation of the property at low temperatures and near the critical region [159]. The proposed equation (41) is given as follows:

$$\omega = \frac{-\ln P_C - 5.92714 + (6.09648/T_{Br}) + 1.28862 \ln T_{Br} + 0.169347\, T_{Br}^6}{15.2518 - (15.6875/T_{Br}) - 13.4721 \ln T_{Br} + 0.43577\, T_{Br}^6}, \tag{41}$$

where $T_{Br} = T_B/T_C$ is the reduced temperature at the boiling point.

Watanasiri et al. developed a correlation to estimate the acentric factor based on heterocyclic compounds and other hydrocarbons and their derivatives [160]. According to their model, the acentric factor is given by the following equation:

$$\omega = \left[0.92217 \times 10^{-3}\, T_B + 0.507288 \frac{T_B}{\mathrm{MW}} + \frac{382.904}{\mathrm{MW}} + 0.242 \times 10^{-5} \left(\frac{T_B}{\mathrm{SG}}\right)^2 - 0.2165 \times 10^{-4}\, T_B \times \mathrm{MW} + 0.1261 \times 10^{-2}\, \mathrm{SG} \right.$$
$$\left. \times \mathrm{MW} + 0.1265 \times 10^{-4}\, \mathrm{MW}^2 + 0.2016 \times 10^{-4}\, \mathrm{SG} \times \mathrm{MW}^2 - 80.6495 \frac{T_B^{1/3}}{\mathrm{MW}} - 0.3738 \times 10^{-2} \frac{T_B^{2/3}}{\mathrm{SG}^2} \right] \left(\frac{T_B}{\mathrm{MW}}\right), \tag{42}$$

where SG is the specific gravity of the component. Values of specific gravity were obtained from the NIST database.

According to Poling et al. [155], the most accurate technique to obtain an unknown acentric factor is from the critical temperature and pressure combined with the normal boiling point. They have found that the most reliable method is given as follows:

$$\omega = -\frac{\ln(P_C/1.01325) + f^{(0)}}{f^{(1)}}, \tag{43}$$

where the critical pressure is in bar and the functions $f^{(0)}$ and $f^{(1)}$ are defined as functions of T_{Br}. These functions are obtained according to the equations proposed by Ambrose and Walton [161]:

$$f^{(0)} = \frac{-5.97616\,(1 - T_{Br}) + 1.29874\,(1 - T_{Br})^{1.5} - 0.60394\,(1 - T_{Br})^{2.5} - 1.06841\,(1 - T_{Br})^5}{T_{Br}}, \tag{44}$$

$$f^{(1)} = \frac{-5.03365\,(1 - T_{Br}) + 1.11505\,(1 - T_{Br})^{1.5} - 5.41217\,(1 - T_{Br})^{2.5} - 7.46628\,(1 - T_{Br})^5}{T_{Br}}. \tag{45}$$

The method proposed by Chen et al. requires the same properties for the estimation of the acentric factor. However, this work suggested a correlation based on the Antoine Equation [157]. Based on 217 compounds over the broadest possible range of T_{Br}, the acentric factor can be estimated as follows:

$$\omega = \frac{0.3\,(0.2803 + 0.4789\, T_{Br}) \log P_C}{(1 - T_{Br})(0.9803 - 0.5211\, T_{Br})} - 1. \tag{46}$$

Furthermore, Constantinou et al. proposed a method for the estimation of the acentric factor using group contribution [162]. The equation for the property estimation is reported as follows:

$$\exp\left(\frac{\omega}{0.4085}\right)^{0.5050} = \sum_i N_i \omega_{1i} + \sum_i M_j \omega_{2j} + 1.1507, \tag{47}$$

where ω_{1i} is the contribution of the first-order group type i occurring N_i times and ω_{2j} is the contribution of the second-order group type j occurring M_j times. The coefficients to determine the acentric factor can be found in Tables A2 and A3 of the Supplementary Material.

4.4.2. Acentric Factor Estimation Results. Estimated values of the acentric factor are given in Table 22.

Figure 9 presents the relative deviation between the different methods when compared to the NIST values, while Table 23 shows the minimum and maximum absolute relative deviation for each method when compared with the data provided by NIST.

The acentric factor provided by NIST is obtained from the Pitzer correlation. The relative deviation concerning the components C20:1 and C24:1 is higher for the methods proposed by Watanasiri et al. and Constantinou et al. This occurs since the estimation of the vapor pressure was not available in the NIST database. Therefore, the NIST values of

TABLE 22: Comparison of experimental and estimated acentric factor.

CN : DB	NIST	Pitzer et al. [158]	Lee and Kesler [159]	Watanasiri [160]	Ambrose and Walton [161]	Chen et al. [157]	Constantinou et al. [162]
C8 : 0	0.782	0.782	0.790	0.493	0.776	0.776	0.780
C10 : 0	0.749	0.749	0.725	0.495	0.709	0.712	0.861
C12 : 0	0.879	0.879	0.889	0.532	0.869	0.872	0.940
C14 : 0	0.940	0.940	0.965	0.605	0.940	0.946	1.017
C16 : 0	0.970	0.970	0.942	0.714	0.917	0.925	1.093
C18 : 0	1.029	1.029	1.001	0.863	0.973	0.984	1.167
C20 : 0	1.184	1.184	1.206	1.031	1.171	1.187	1.239
C22 : 0	1.233	1.233	1.252	1.243	1.215	1.234	1.310
C24 : 0	0.810	0.810	1.449	1.508	1.403	1.437	1.379
C16 : 1	1.088	1.088	1.105	0.751	1.075	1.084	1.079
C18 : 1	1.247	1.345	1.342	0.856	1.304	1.315	1.153
C20 : 1	0.725	—	0.742	1.184	0.719	0.736	1.226
C22 : 1	1.080	1.080	1.102	1.294	1.068	1.091	1.297
C24 : 1	0.676	—	0.694	1.766	0.671	0.694	1.366
C18 : 2	0.996	0.956	0.945	1.043	0.920	0.929	1.140
C18 : 3	1.022	0.976	0.950	1.054	0.922	0.936	1.127
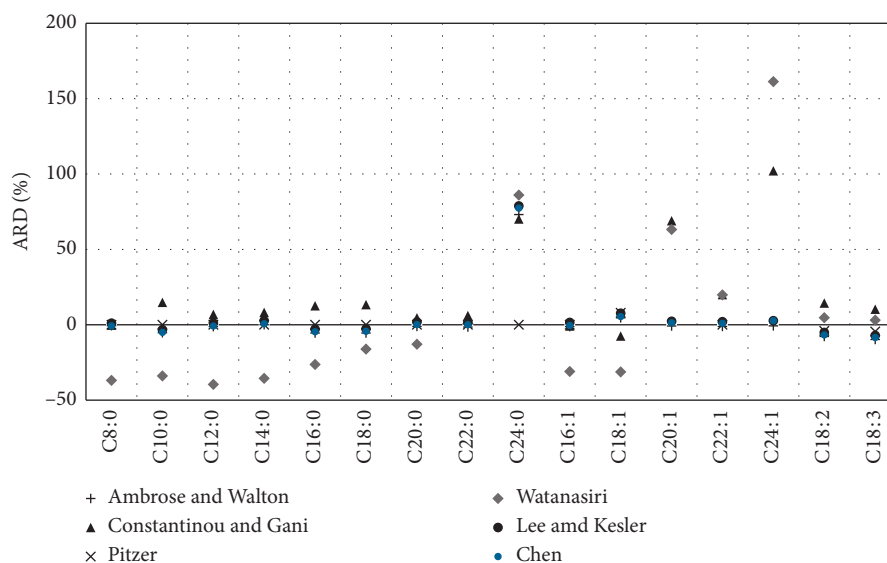
FIGURE 9: Absolute relative deviation of estimation of the acentric factor.

the acentric factor for these two components were probably estimated using another method. In addition, the acentric factor of the component C24 : 0 is inconsistent when compared to the other saturated fatty acids, which makes this value doubtful. Once the Pitzer equation was used for the estimation of the values from NIST, the absolute deviation of Pitzer regarding the NIST acentric value is negligible.

The method proposed by Watanasiri et al. reported a higher deviation with respect to NIST. This is due to the fact that, in their study, the correlations were built using a different set of components that did not include fatty acids. Followed by this method, Constantinou et al. reported the second-highest deviation since their estimation was made by using the group contributions instead of the physical properties of the components. Conversely, the methods by Lee and Kesler, Ambrose and Walton, and Chen et al. have reported low deviation compared to NIST.

The acentric factor has a definition based on vapor pressure. In this way, the property is indirectly measured, which can result in uncertainties in the estimation. The estimation of the acentric factor for the unsaturated fatty acids as well as the component C24 : 0 reported some inconsistencies. Disregarding those fatty acids, the average absolute relative deviation of the methods reduced to 0% for Pitzer et al., 2.1% to Lee and Kesler method, 25.3% for Watanasiri, 2.6% for Ambrose and Walton, 2.1% for Chen et al., and 8.4% for the method proposed by Constantinou et al. Therefore, these estimations are more reliable for the saturated fatty acids from C8 : 0 to C22 : 0.

4.4.3. Novel Acentric Factor Estimation Method. The novel method proposed to estimate the acentric factor is given as follows:

TABLE 23: Deviations of different methods for the prediction of the acentric factor.

	Pitzer et al. [158]	Lee and Kesler [159]	Watanasiri [160]	Ambrose and Walton [161]	Chen et al. [157]	Constantinou et al. [162]
AAD (K)	0.01	0.07	0.32	0.07	0.07	0.19
RMSD (K)	0.03	0.16	0.41	0.15	0.16	0.27
AARD (%)	1.2	7.8	37.7	7.5	7.5	22.6
MIN RD (%)	−4	−7	−40	−10	−8	−7
MAX RD (%)	8	79	161	73	77	102

TABLE 24: Coefficients for the estimation of the acentric factor (valid from C8:0 to C22:0) according to equation (48).

Coefficients	Values
$A_{\omega_{\mathrm{FA\,CN}:n}}$	$5.4382E-05$
$B_{\omega_{\mathrm{FA\,CN}:n}}$	-0.0032
$C_{\omega_{\mathrm{FA\,CN}:n}}$	6.4600
$\alpha_{\omega\mathrm{CN}:0}$	0.1066

TABLE 25: Coefficients for the estimation the temperature nondependent properties according to equation (49).

Coefficients	T_B	T_M	T_C	P_C	V_C	ω
A	$-7.0670E-04$	$-4.1905E-04$	$-1.8345E-03$	$7.0357E-04$	$-1.0023E-06$	$5.4382E-05$
B	0.9173	0.4863	1.6239	-0.5776	0.0206	-0.0032
C	205.6120	193.9418	550.5882	143.4049	-0.9068	6.4600
$\alpha_{\mathrm{CN}:0}$	1.5697	1.1380	0.9286	0.3515	0.2485	0.1066
$\alpha_{\mathrm{CN}:1}$	1.5501	0.9752	0.9185	0.3556	0.2106	—
$\alpha_{\mathrm{CN}:2}$	1.5323	0.8999	0.9134	0.3836	0.2033	—
$\alpha_{\mathrm{CN}:3}$	1.5329	0.8759	0.9028	0.3323	0.2025	—

$$\omega = \alpha_{\omega\,\mathrm{CN}:n} \times \left[A_{\omega\,\mathrm{FA}}\,(MW)^2 + B_{\omega\,\mathrm{FA}}\,(MW) + C_{\omega\,\mathrm{FA}} \right]. \tag{48}$$

The coefficients $A_{P_{C_{\mathrm{FA\,CN}:n}}}$, $B_{P_{C_{\mathrm{FA\,CN}:n}}}$, $C_{P_{C_{\mathrm{FA\,CN}:n}}}$, and $\alpha_{P_M\mathrm{CN}:n}$ were obtained by minimizing the relative deviations between the values estimated by the novel method and the NIST database values, using the GRG nonlinear solving method to achieve the optimized result.

As the variability of the NIST database is very high, mainly for the unsaturated fatty acids, the novel method will be only valid to estimate the acentric factors for fatty acids within the range between C8:0 and C22:0. The coefficients to determine the acentric factor are provided in Table 24.

For the novel method for the acentric factor, AAD = 0.03 K, RMSD = 0.03 K, AARD = 3.0%, MIN RD = −3.0%, and MAX RD = 7.1%.

5. Conclusions

Over one hundred biomass sources were reviewed, and 16 saturated, unsaturated, and polyunsaturated fatty acids were selected, based on their frequency and amount. The selected saturated fatty acids ranged from C8 to C24, in agreement with Kenar et al. [163], which states that "*saturated fatty acids having alkyl chain lengths greater than 18 carbon atoms are often negligible in most seed oils and are only found at useful levels in a few unusual seed oils.*"

Different unsaturated fatty acids with 1, 2, or 3 double bonds were considered.

Among the saturated fatty acids, the highest average yields were found for palmitic (C16:0) and stearic (C18:0) acids, with a value of around 15 and 5%, respectively. The highest yields for the unsaturated fatty acids were found for oleic (C18:1), linoleic (C18:2), and linolenic (C18:3) acids, at around 32, 27, and 7%, respectively. The frequency of palmitic (C16:0), stearic (C18:0), oleic (C18:1), and linoleic (C18:2) acids is around 100% since almost all the selected biomasses have these four fatty acids.

Available estimation methods for the temperature nondependent properties, such as normal boiling point, normal melting point, critical properties, and acentric factor, were compared, and novel estimation methods were developed to enhance their predictions. The novel proposed method is simple to use, and it is based on the molecular weight and the maximum number of double bonds in the molecule. This method is generalized in equation (49), where PP is the temperature nondependent physical property:

$$\mathrm{PP} = \alpha_{\mathrm{CN}:n} \cdot \left[A\,(MW)^2 + B\,(MW) + C \right]. \tag{49}$$

The three coefficients, assigned as A, B, and C, and the correction factor $\alpha_{T_B\mathrm{CN}:n}$, which depends on the number of unsaturation, are summarized in Table 25.

For all the properties, new equations provide a better estimation with an absolute average deviation equal to or

lower than 4.6%, compared to the values of the NIST database used as reference. This approach allows a better fatty acid property prediction compared to other previously published methods.

It should be highlighted that the classic group contribution methods have been developed to be applied to a wide range of chemical compounds and different research groups implemented various corrections to take into account the possible interaction between different molecule fragments. However, the validity of the equations developed in this work is limited for the fatty acids selected.

The equations proposed represent an improvement in the modelling of processes related to the recovery and purification of fatty acids from biomasses. Indeed, these equations have the potential to become a stepping stone for investigations of fatty acid mixtures or triglycerides [4], taking into account that the first step in process modelling relies on accurately predicting their physical properties.

Data Availability

The data used to support the findings of this study are included within the supplementary information file.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Acknowledgments

Supplementary Materials

The Supplementary Material included together with the submission reports the data used for the physical properties calculation with the methods described in the article. The contributions for the estimation methods considered used to support the findings of this study are included within the supplementary information file. (*Supplementary Materials*)

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