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Using Two Group-Contribution Methods to Calculate Properties of Liquid Compounds Involved in the Cyclohexanone Production Operations

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Abstract: A numerical application has been carried out to determine the thermophysical properties of more than fifty pure liquid compounds involved in the production process of cyclohexanone, whose real values are unknown, in many cases. Two group-contribution methods, the Joback and the Marrero–Gani methods, both used in the fields of physicochemistry and engineering, are employed. Both methods were implemented to evaluate critical properties, phase transition properties, and others, which are required for their use in industrial process simulation/design. The quality of the estimates is evaluated by comparing them with those from the literature, where available. In general, both models provide acceptable predictions, although each of them shows improvement for some of the properties considered, recommending their use, when required.

Keywords: cyclohexanone; group-contribution methods; Joback method; Marrero–Gani method

Citation: Fernández, L.; Ortega, J.; Domínguez, L.; Lorenzo, D.; Santos, A.; Romero, A. Using Two Group-Contribution Methods to Calculate Properties of Liquid Compounds Involved in the Cyclohexanone Production Operations. *Liquids* **2022**, *2*, 413–431. https://doi.org/10.3390/liquids2040024

Academic Editor: Enrico Bodo

Received: 31 October 2022
Accepted: 18 November 2022
Published: 23 November 2022

1. Introduction

In a previous work [1], an exhaustive analysis was carried out on the possibilities of the separation of a set of substances generated in the production process of cyclohexanone, the base compound for the manufacture of nylon-6, used in the textile industry. However, the indicated process is not direct, intermediate processes being necessary to obtain ε-caprolactam, a precursor of nylon-6. Therefore, the production of cyclohexanone as a raw material for different industrial processes, including different types of nylon, is high, currently at approximately 6 MTm/year [2]. In addition, the quality requirements of the cyclic ketone are also high, and the purification process from cyclohexane is complex, as shown in Figure 1. This makes it necessary to optimize the different separation stages, both technically and economically, whose performance represents an important area of work in the field of chemical engineering, requiring an appropriate modeling with the support of the mathematics-thermodynamics binomial.

According to Figure 1, cyclohexanone is obtained by the oxidation of cyclohexane, producing, in addition to cyclohexanone, cyclohexanol, cyclohexyl hydroperoxide, and many other compounds, in smaller proportion. The last-mentioned compound is reconverted (after washing with water and alkalis) into the first two, after removing undesirable compounds by decantation. The resulting solution is subjected to distillation, separating the unreacted cyclohexane in the first unit and recycled into the initial process unit, while the cyclohexanol is dehydrogenated to convert it to cyclohexanone. The aforementioned operations, as defined, suggest a simple development of the global process; however, the current development of the process is quite different due to the formation, during the different stages, of many compounds (more than fifty, although they are considered secondary) that are produced from the beginning with the oxidation of cyclohexane, and in varying quantities, some of them unidentified up until now [3–10].

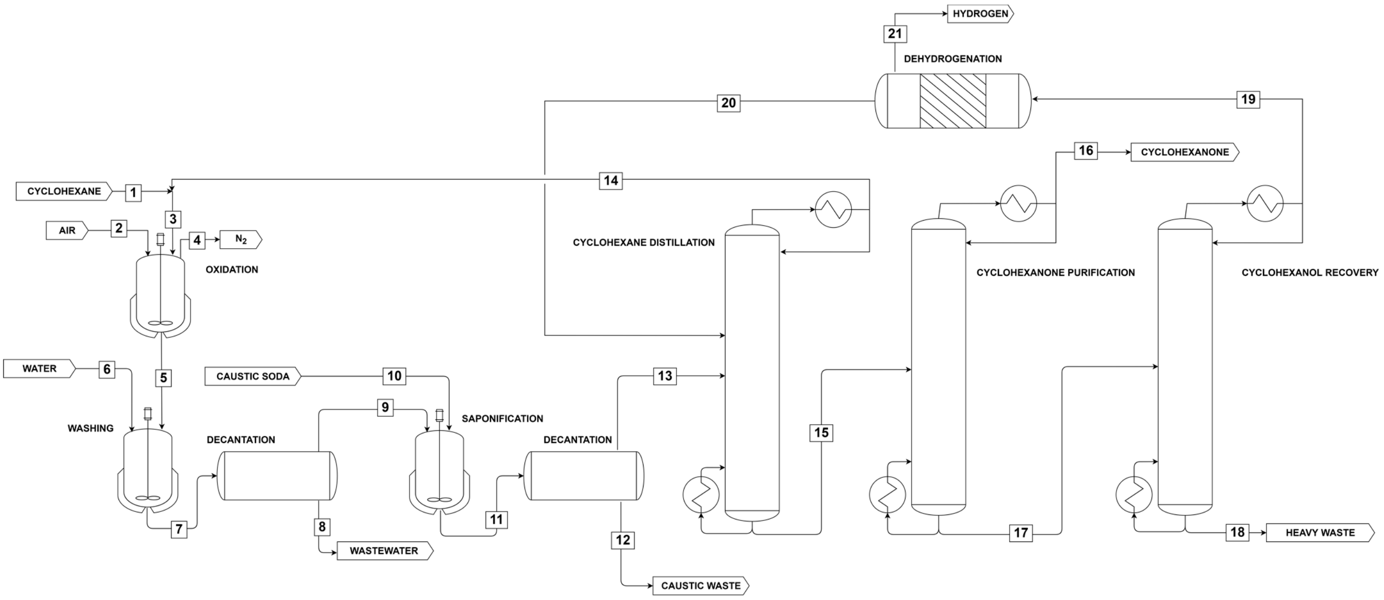


Figure 1. Scheme indicating the different operation units existing in the cyclohexanone production process.

Many of the compounds discovered in various cyclohexanone production plants are shown in Appendix A, indicating the process streams in which they are found. Some of these substances do not pose a problem for the quality of cyclohexanone, either because they are easy to separate, e.g., cyclohexane (streams 1, 3, 5, 7, 9, 11) or cyclohexylidene-cyclohexanone (stream 16), see Figure 1, or because they are only present when the process operates outside its normal conditions, such as 5-hexenal (stream 19 in Figure 1). However, other substances are likely to contaminate cyclohexanone, creating the need to design appropriate separation operations to remove the most undesirable substances. Appendix B shows a list of substances that influence the global process, including some common substances, such as phenol and toluene, as well as many others that are unusual and little studied, whose properties are unknown. In any case, the design of separation processes depends on the availability of the physicochemical information for the substances involved, as well as their solutions. The most important information required, such as boiling temperatures, enthalpies of change of state, thermal capacities, and critical properties, among others, are used to define the corresponding operation units.

The necessary information is obtained through direct experimentation and with appropriate equipment; however, these actions are costly, both in terms of money and time. Without ignoring the importance of experimental work, in the chemical engineering field, the theoretical estimation methods are sometimes used to generate approximate values of the properties involved in the design of operations. In the literature [11–15], there are many methods for estimating the thermophysical properties of pure substances and solutions; of these, the so-called "group contribution methods" (GCM) prove to be useful and easy to use in practical engineering cases. A GCM is generated as a mathematical tool that combines the particular contributions of each of the functional groups present in the molecules of a compound/system to the calculation of a given thermophysical property. In a previous work [1], the Joback method [14] was used to discriminate between positional isomers, but an exhaustive assessment of the reliability of the estimates was not performed.

Once the necessity of certain properties of a large number of substances—more than fifty involved in the global process, shown in Figure 1—is known, the goal of this work is to estimate these requirements to achieve the process design. For this, two GCM procedures were used: the Joback, previously mentioned, and the Marrero–Gani [15], checking the results to determine their reliability given the different levels of theory of both methodologies, which will be quantified by comparing the predicted results with the values available in the literature.

2. Two Group-Contribution Methods for Estimating Properties of Pure Substances

The GCMs are based on the assumption that the properties of a chemical compound can be calculated by combining, by means of certain procedures (differeing according to the method), the contribution to that property of the different "fragments" that make up its molecule. To do this, the molecule is broken down using "standardized" entities or "groups", varying depending on the method. To each group (see Figures 2 and 3) is assigned a numerical parameter that quantifies its contribution to the studied property. This approach makes it possible to calculate the properties of a substance by determining the number of groups of each type present in the molecule and then applying a simple calculation defined by the corresponding method. In the first-order GCMs, the contribution of each group is assumed to be independent of its environment and of other groups. Therefore, by using experimental data of the compounds containing that group, the contribution of the parameter associated with it can be determined. In this way, the values obtained can be used to estimate the properties of other substances for which experimental information is not available.

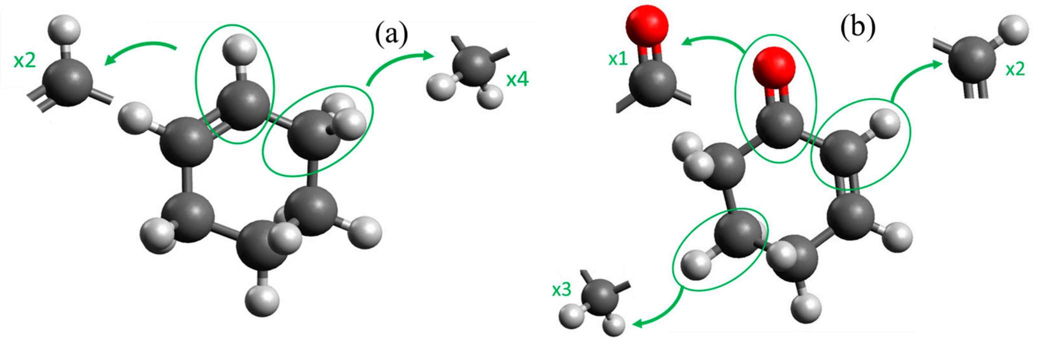


Figure 2. Decomposition of molecules according to the Joback method [14]. (**a**) Cyclohexene, (**b**) 2-cyclohexen-1-one.

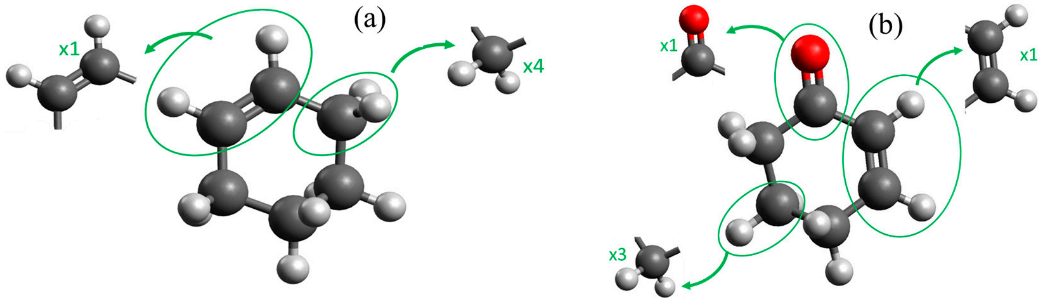


Figure 3. Decomposition of molecules according to Marrero–Gani method [15]. (**a**) Cyclohexene, (**b**) 2-cyclohexen-1-one.

One of the best known first-order methods for estimating the properties of pure substances is the Joback [14] method used in this work, since it has been shown to produce estimates with acceptable accuracy and, in addition, it can be applied to a wide variety of groups and properties, characteristics that justify its relevance as a tool in chemical engineering calculations.

The major drawback of the Joback method, and also of others classified as first-order methods, is that they do not differentiate the calculation for the case of molecules constituting the so-called position isomers. These methods are also unsuitable for complex molecules for which the chemical environment significantly influences the thermophysical behavior. These deficiencies are corrected by the higher-order qualified methods, as they include additional groups produced by combinations of lower-order groups, and whose parameters take into account the effect caused by the chemical environment. Marrero and Gani [15] developed a method that includes groups of several levels (specifically three), producing acceptable results. Therefore, this method, along with the Joback method, is used in this work to determine the properties of the selected compounds, as described briefly in the following section, with examples illustrating the specific calculation procedures.

2.1. The Joback Method

In this procedure, the contributions of the groups generate a parameter in a characteristic equation defined for each property with which the estimation is achieved. The authors [14] provide equations for different thermophysical quantities, such as boiling temperatures T_b^o, melting temperatures T_m^o, enthalpies of changes of state, vaporization enthalpies Δh_v^o, melting enthalpies Δh_m^o, enthalpies of formation Δh_f^o, Gibbs energy formation Δg_f^o, isobaric thermal capacities, c_p, and critical properties; p_c, v_c, T_c. Table A1 of Appendix C compiles the calculation equations for each of these properties, showing the characteristic parameters of the groups of each property in the second column of the table, whose values are quantified [14]. To estimate the molecule's properties, it is broken down into the groups identified by Joback [14], as shown in Figure 2, with two specific cases taken as examples: cyclohexene and 2-cyclohexen-1-one. Once the groups have been identified and quantified, this method multiplies the parameter of each group by adding the value obtained for all the groups. With these values, the property is estimated using the expressions shown in the third column of Table A1. Table 1 shows the values obtained for the critical properties of the two species chosen in Figure 2, comparing the results with those from the literature, as indicated.

Table 1. Groups for cyclohexene and 2-cyclohexen-1-one, according to Joback method [14], and the contribution terms for critical properties. N_k is the number of groups in the molecules; $\tau_{c,k}$, $\pi_{c,k}$, $v_{c,k}$ are the contributing parameters corresponding to T_c, p_c, and v_c, respectively. The calculated values and those estimated by the procedure are shown.

Compounds	**Groups**	N_k	$\tau_{c,k}$	$\pi_{c,k}$	$v_{c,k}$
Cyclohexene	$-CH_2-$	4	0.0100	0.0025	48
	$=CH-$	2	0.0082	0.0011	41
	total:		0.0564	0.0122	274
	estimated→		$T_c/K = 567$	$p_c/bar = 43.3$	$v_c/cm^3 \cdot mol^{-1} = 291$
	from ref. [16]		$T_c/K = 560.4$	$p_c/bar = 48.41$	$v_c/cm^3 \cdot mol^{-1} = 377.4$
2-Cyclohexen-1-one	$-CH_2-$	3	0.0100	0.0025	48
	$=CH-$	2	0.0082	0.0011	41
	$>C=O$	1	0.0284	0.0028	55
	total:		0.0784	0.0125	281
	estimated→		$T_c/K = 655$	$p_c/bar = 45.3$	$v_c/cm^3 \cdot mol^{-1} = 298$
	from ref. [17]		$T_c/K = 685.0$	$p_c/bar = 45.30$	$v_c/cm^3 \cdot mol^{-1} = 304.9$

2.2. Marrero–Gani Method

This procedure [15], pointed out in the previous section as of higher order, uses groups in three different orders. The first-order groups correspond to those with a single functional group and divide the molecule into fragments similar to those used in the Joback method, e.g., linear alkanes and monofunctional compounds. Second-order groups are used to improve the estimation of branched and polyfunctional compounds, with a maximum of one aromatic ring; these groups are established by combining two or more functional groups. Lastly, third-order groups are used to represent polycyclic compounds and specific combinations of functional groups, allowing the method to make satisfactory estimates of complex molecules. As in the Joback method, the Marrero–Gani method allows the same properties to be estimated, with the exception of the isobaric thermal capacity. The corresponding mathematical equations of this procedure are presented in Appendix D.

The application of the method to the same compounds chosen as examples in Section 2.1 requires the generation of the groups in the molecules. Figure 3a shows that those with first-order groups corresponding to cyclohexene coincide with those in the Joback method (Figure 2a), with the addition of the second-order groups. However, 2-cyclohexen-1-one is a polyfunctional compound, containing both first- and second-order groups, as shown in Figure 2b. Table 2 shows the results obtained with the application of the Marrero–Gani method to the estimation of the critical properties of the two selected molecules, comparing the results with those from the literature.

Table 2. Groups for cyclohexene and 2-cyclohexen-1-one, according to Marrero–Gani method [15], and contribution parameters for critical properties. N_k is the number of groups in the molecules, and j is the group order. Calculated values and those estimated by the procedure are shown.

Compounds	Groups	j	N_k	$T_{c,i,j}$	$p_{c,i,j}$	$v_{c,i,j}$
Cyclohexene	CH_2 (cyc)	1°	4	1.8815	0.009884	49.24
	CH=CH (cyc)	1°	1	3.6426	0.013815	83.91
	total:			11.1686	0.053351	280.87
	estimated→			T_c/K = 558	p_c/bar = 43.9	$v_c/\text{cm}^3\cdot\text{mol}^{-1}$ = 289
	from ref. [16]			T_c/K = 560.4	p_c/bar = 48.41	$v_c/\text{cm}^3\cdot\text{mol}^{-1}$ = 377.4
2-Cyclohexen-1-one	CH_2 (cyc)	1°	3	1.8815	0.009884	49.24
	CH=CH (cyc)	1°	1	3.6426	0.013815	83.91
	CO (cyc)	1°	1	12.6396	−0.000207	57.38
	total:			21.9267	0.043260	289.01
	estimated→			T_c/K = 714	p_c/bar = 49	$v_c/\text{cm}^3\cdot\text{mol}^{-1}$ = 297
	from ref. [17]			T_c/K = 685.0	p_c/bar = 45.30	$v_c/\text{cm}^3\cdot\text{mol}^{-1}$ = 304.9

3. Evaluation of Estimates for the Selected Substances

The numerical results obtained for the different properties for all the compounds selected, estimated with the Joback and Marrero–Gani methods, are given in Appendix C (Table A2) and Appendix D (Table A5), respectively. A comparison with the values available in the literature is made in this section.

3.1. Evaluation of Temperatures and Enthalpies of Phase Transition

Figure 4a compares the values found [16–30] for the boiling temperatures, T_b^o, and the estimates obtained by both methods, showing the existence of a direct correlation. The Joback method produces greater dispersion in the results than does the Marrero–Gani method, which is reflected in a lower R^2 coefficient. The residuals yield an average error of 2.2% for the Joback method, and a slightly lower average error of 0.6% for the Marrero–Gani method, the average standard deviation of the former, 12.5 K, being higher than that of the latter, 4.5 K.

Figure 4b shows the comparison of the estimates made using both methods for the melting temperatures, T_m^o, in relation to the values found in the literature [16,23,24,29–40]. In general, both methods present estimates with a lower order than the T_b^o, the average errors for both methods being close to 9%, with average standard deviations of 32 K for the Joback method and 25 K for the Marrero–Gani method.

Figure 5a compares the estimates of enthalpies of vaporization, Δh_v^o with the literature values [16,20,24,41–48]. Both methods yield similar results, with average errors of 15.3%, for the Joback method, and 19.7%, for the Marrero–Gani method. The similarity is greater for the case of melting enthalpies, Δh_m^o [16,30,31,46–50], Figure 5b, yielding average error values of 15.9%, with Marrero–Gani method, and 16.9%, with the Joback method. However, in both cases, the determination coefficient for the melting enthalpy is very small.

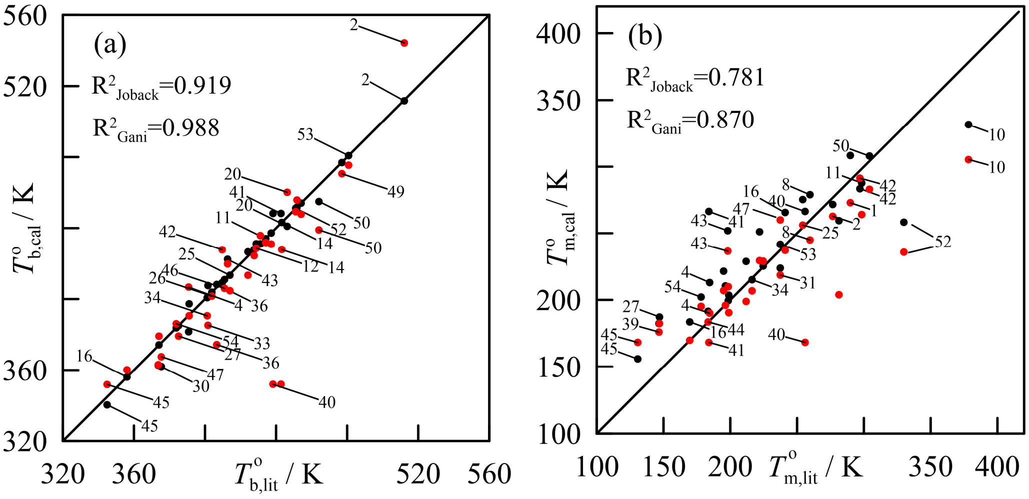


Figure 4. (**a**) Comparison between the boiling temperatures, $T^{o}_{b,lit}$, from literature and those estimated, $T^{o}_{b,cal}$, by the methods of Joback (🔴) and Marrero–Gani (●). (**b**) Analogous comparison for the melting temperatures. Labels correspond to the order of compounds established in Appendix B.

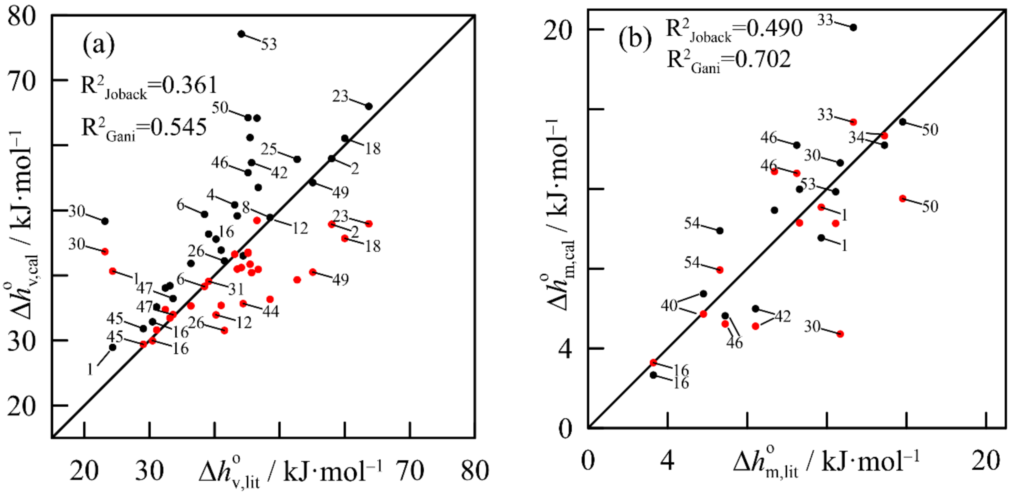


Figure 5. Comparison between the enthalpies of phase transition obtained by the methods of Joback (🔴) and Marrero–Gani (●) and those from the literature: (**a**) vaporization enthalpies; (**b**) melting enthalpies. Labels correspond to the order of compounds, as shown in Appendix B.

3.2. Critical Properties

Comparison with literature data [16,17,24,39,51–57] of the critical temperatures, T_c, is shown in Figure 6a–c, and the estimates are considered acceptable. The two methods show good experimental vs. model correlations; those of the Marrero–Gani method rise to an average error of 3.5%, compared to 2.9% according to the Joback method. In contrast, the critical pressure p_c is slightly better represented by the Marrero–Gani method (5.7%) than by the Joback method (6.2%). The results for the critical volume, v_c, yield errors of 5.9% (Marrero–Gani) and 4.6% (Joback), although the information for this property is currently scarce. Numerical values of all those properties are shown in Tables A2 and A5 of the Appendices C and D.

3.3. Estimation of Enthalpies of Formation and Thermal Capacities

The amount of information available for the enthalpies of formation, Δh^{o}_{f} [16,24,58–67], and thermal capacities, c_p [16,50,64,68–73], is reduced for the set of selected compounds; therefore, the comments made in this work on these properties cannot be assessed generically. The estimation of Δh_f^o is acceptable using both models, as shown in Figure 7a. The average errors are around 12% for the Joback method and much higher—21%—for the Marrero–Gani method. The estimation of the c_ps is only conducted using the Joback method (Figure 7b), with a systematic deviation that underestimates the value of the property with respect to the experimental values, showing an average error of more than 32%.

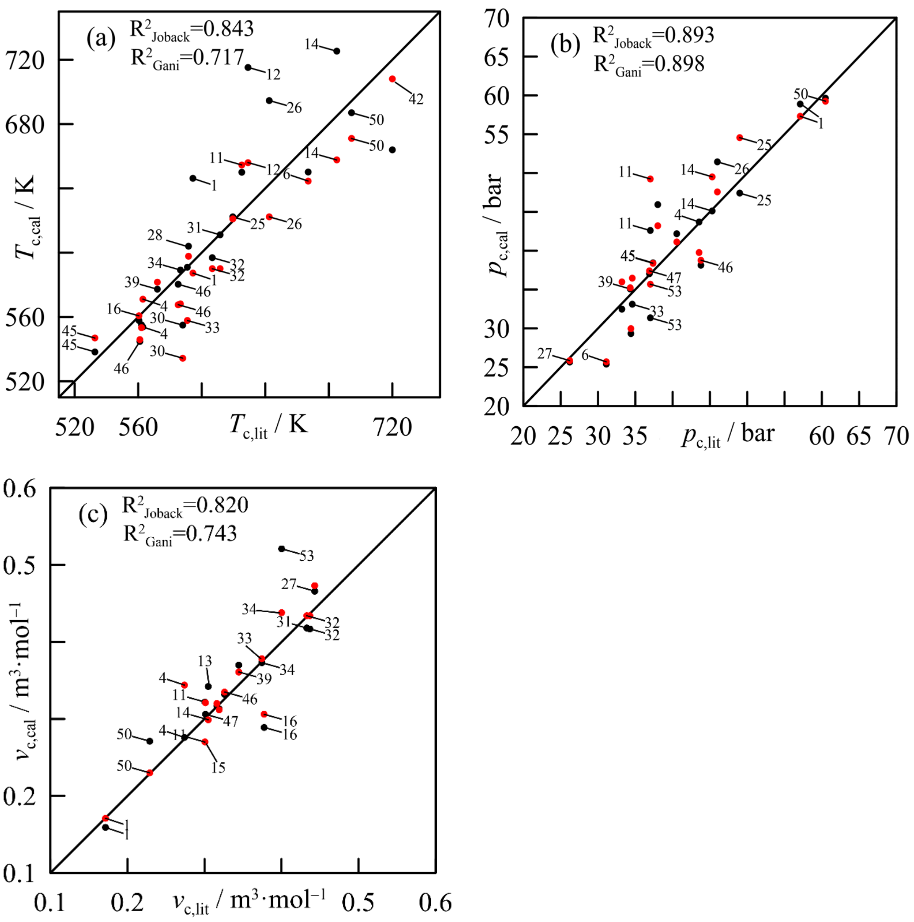


Figure 6. Comparison between the critical properties obtained from the literature and those calculated by the methods of Joback (●) and Marrero–Gani (●): (**a**) critical temperature; (**b**) critical pressure; (**c**) critical volume. Labels correspond to the order of compounds, as shown in Appendix B.

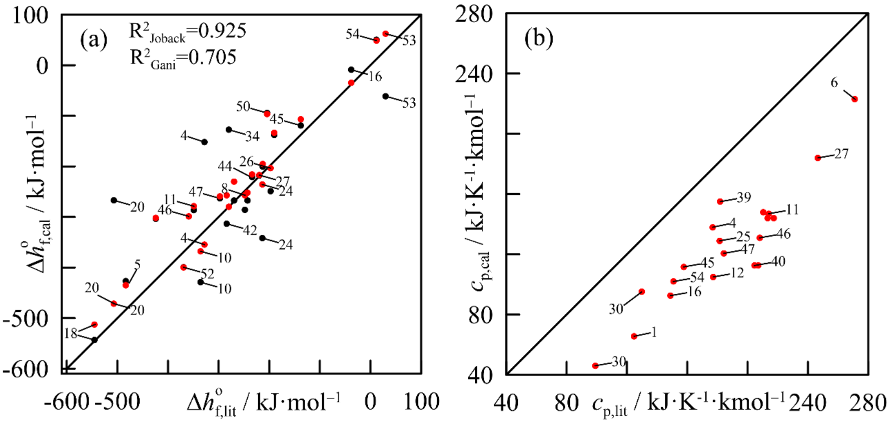


Figure 7. (**a**) Comparison between the enthalpies of formation obtained from literature and those calculated by the methods of Joback (●) and Marrero–Gani (●). (**b**) Comparison between the thermal capacities obtained from literature and those calculated by the Joback method. Labels correspond to the order of compounds, as shown in Appendix B.

4. Conclusions

Estimates are presented for different properties of a set of substances involved in the cyclohexanone production process, as obtained using two group-contribution methods: the Joback method [14] and the Marrero–Gani method [15]. The predictions made are evaluated by comparing the results with those available in the experimental research. The latter does not lead to a clear choice of one method over the other, as the comparisons made do not sufficiently clarify the preference.

The Marrero–Gani method has a higher level of theory, since it uses groups of different orders, which allows it to be used for isomeric compounds. In general, it produces better results for most properties, with the exception of the melting enthalpy, critical temperature, and critical volume, which are better represented by the Joback method. The latter can also be used to estimate thermal capacities. Despite these differences and the assessment of the small errors obtained with both methods, at least statistically, it is acceptable to use either of the two procedures. The major advantage of using the Joback method is that it is simpler, where appropriate.

In summary, the use of any of these methods provides a rapid and reasonably reliable approximation of the different properties required to address a given analysis or simulation in order to optimize the cyclohexanone production process. For a practical case, the methods used have served to estimate boiling temperatures and critical properties, which are important for evaluating the distillation process of the towers shown in Figure 1. Likewise, the approximation obtained for the enthalpies of phase change, especially those of vaporization and thermal capacities, facilitates the design of the heat exchangers, such as the reboilers and condensers of the towers mentioned. The properties corresponding to the enthalpies of formation and the Gibbs energies are involved in the prediction of the complex reactions that take place in the different stages of the global process.

Author Contributions: Conceptualization, J.O., L.F. and A.S.; methodology, L.F. and J.O.; software, L.F.; validation, J.O., A.S., A.R. and D.L.; formal analysis, L.D. and J.O.; investigation, J.O. and L.F.; resources, J.O. and L.F.; data curation, L.F.; writing—original draft preparation, L.F. and J.O.; writing—review and editing, J.O., D.L. and L.F.; visualization, L.F., J.O., L.D., A.S., D.L. and A.R.; supervision, J.O.; project administration, J.O.; funding acquisition, J.O. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The data used and presented in this work were calculated according to Appendices C and D.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Compounds Present in the Streams of the Cyclohexanone Production Process

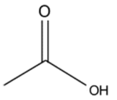
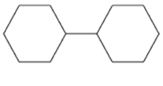
1. Cyclohexane feeding; cyclohexane, hydrocarbons.
2. Oxidant supply; air.
3. Entrance to oxidation; cyclohexane, hydrocarbons, cyclohexanone, cyclohexanol, light oxides.
4. Nitrogen.
5. Oxidation effluent; cyclohexane, cyclohexanone, cyclohexanol, light and heavy oxidized, peroxides, formic acid, acetic acid, other monocarboxylic acids, dicarboxylic acids, esters, butanol, pentanol, cyclopentanone, cyclopentanol, 2-pentanone, 2-cyclo-hexen-1-one, cyclohexene, 2-methylcyclopentanone, methylcyclopentanol, heptanones, 2-methyl-3-heptanone, 1,3-cyclohexanedione, 1,2-cyclohexanediol, methylcyclohexanols, ethers.
6. Washing water; water.
7. Washing emulsion; water, cyclohexane, cyclohexanone, cyclohexanol, light and heavy oxidized, peroxides, formic acid, acetic acid, other monocarboxylic acids, dicarboxylic acids, esters, butanol, pentanol, cyclopentanone, cyclopentanol, 2-pentanone, 2-cyclo

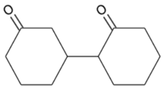
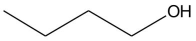
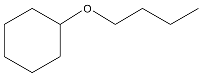
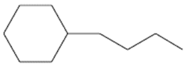
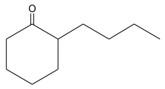
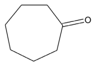
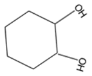
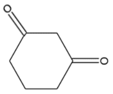
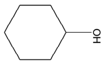
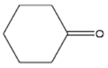
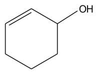
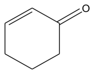
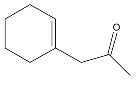
hexen-1-one, cyclohexene, 2-methylcyclopentanone, 1-methylcyclopentanol, heptanones, 2-methyl-3-heptanone, 1,3-cyclohexanedione, 1,2-cyclohexanediol, methylcyclohexanols, ethers.

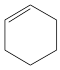
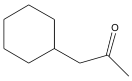
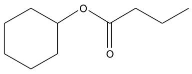
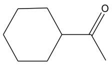
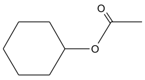
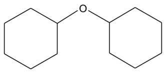
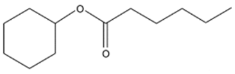
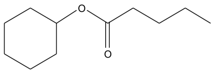
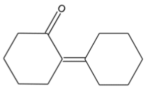
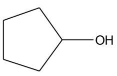
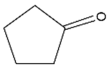
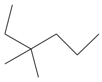
8. Acid water; water, formic acid, acetic acid, other monocarboxylic acids.
9. Oxidized product; cyclohexane, cyclohexanone, cyclohexanol, light and heavy oxidized, peroxides, monocarboxylic acids, dicarboxylic acids, esters, butanol, pentanol, cyclopentanone, cyclopentanol, 2-pentanone, 2-cyclohexen-1-one, cyclohexene, 2-methyl cyclopentanone, 1-methylcyclopentanol, heptanones, 2-methyl-3-heptanone, 1,3-cyclo hexanedione, 1,2-cyclohexanediol, methylcyclohexanols, ethers.
10. Alkali; water, sodium hydroxide.
11. Saponification emulsion; water, sodium hydroxide, cyclohexane, cyclohexanone, cyclohexanol, light and heavy oxidized, peroxides, monocarboxylic acids, dicarboxylic acids, esters, butanol, pentanol, cyclopentanone, cyclopentanol, 2-pentanone, cyclohexenone, cyclohexene, methylcyclopentanone, methylcyclopentanol, heptanones, methylheptanone, cyclohexanedione, cyclohexanediol, methylcyclohexanols, ethers.
12. Sodium salts; sodium hydroxide, sodium salts.
13. Saponified product; sodium hydroxide, cyclohexanone, cyclohexanol, light oxidized.
14. Cx I recycle; cyclohexanone, cyclohexanol, light oxides.
15. KA-Oil; cyclohexanone, cyclohexanol, oxides, alcohols, aldehydes and ketones.
16. Purified cyclohexanone; butanol, pentanol, cyclopentanol, cyclopentanone, 5-hexenal, hexanal, 2-hexanone, cyclohexanone, cyclohexanol, 2-cyclohexen-1-one, heptanones, methylcyclohexanones, butylcyclohexane, cyclohexyl-butyl-ether.
17. Residue from the purification of cyclohexanone; cyclohexanol, 2-cyclohexen-1-one, 2-cyclohexen-1-ol, heptanones, methylcyclohexanones, butylcyclohexane, cyclohexyl-butyl-ether, cyclohexene oxides, cyclohexylidene-cyclohexanone, cyclohexanone oligo mers, pentylcyclohexane, cyclohexyl acetate, other light/heavy condensation products.
18. Heavy-residue; cyclohexylidene-cyclohexanone, cyclohexanone oligomers, heavy condensation products.
19. Cyclohexanol for dehydrogenation; cyclohexanone, cyclohexanol, 2-cyclohexen-1-one, 2-cyclohexen-1-ol, heptanones, methylcyclohexanones, butylcyclohexane, cyclohexyl-butyl-ether, cyclohexene oxides, cyclohexylidene-cyclohexanone, cyclohexa-none oligomers, n-pentylcyclohexane, cyclohexyl acetate, other light/heavy condensation products.
20. Cyclohexanol recycle; cyclopentanol, hexanal, 2-hexanone, cyclohexanone, cyclohexanol, cyclohexenone, cyclohexenol, heptanones, methylcyclohexanone, cyclohexyl-butyl ether.
21. Hydrogen.

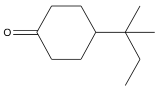
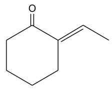
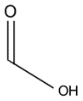
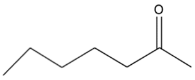
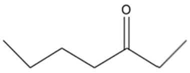
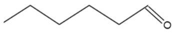
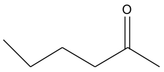
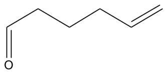
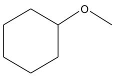
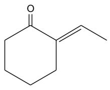
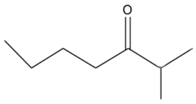
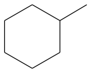
Appendix B. Compounds Involved in the Production Process of Cyclohexanone

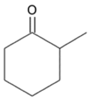
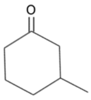
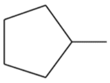
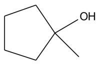
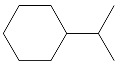
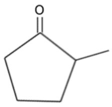
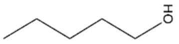
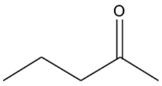
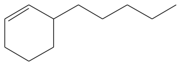
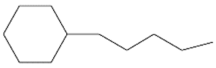
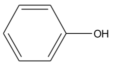
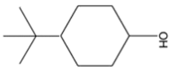
Order number, compound, empirical formula, structure, and CAS number are indicated.

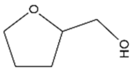
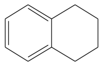
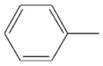
No.	Compound	Formula	Chemical Structure	CAS#
1	acetic acid	$C_2H_4O_2$		64-19-7
2	1,1′-bicyclohexyl	$C_{12}H_{22}$		92-51-3

No.	Compound	Formula	Chemical Structure	CAS#
3	[1,1′-bicyclohexyl]-2,3′-dione	$C_{12}H_{18}O_2$		55265-34-4
4	1-butanol	$C_4H_{10}O$		71-36-3
5	butoxycyclohexane	$C_{10}H_{20}O$		24072-44-4
6	butylcyclohexane	$C_{10}H_{20}$		1678-93-9
7	2-butylcyclohexanone	$C_{10}H_{18}O$		1126-18-7
8	cycloheptanone	$C_7H_{12}O$		502-42-1
9	1,2-cyclohexanediol	$C_6H_{12}O_2$		931-17-9
10	1,3-cyclohexanedione	$C_6H_8O_2$		504-02-9
11	cyclohexanol	$C_6H_{12}O$		108-93-0
12	cyclohexanone	$C_6H_{10}O$		108-94-1
13	2-cyclohexen-1-ol	C_6H_8O		822-67-3
14	2-cyclohexen-1-one	C_6H_8O		930-68-7
15	1-(1-cyclohexen-1-yl)-2-propanone	$C_9H_{14}O$		768-50-3

No.	Compound	Formula	Chemical Structure	CAS#
16	cyclohexene	C_6H_{10}		110-83-8
17	cyclohexyl acetone	$C_9H_{16}O$		103-78-6
18	cyclohexyl butanoate	$C_{10}H_{18}O_2$		1551-44-6
19	cyclohexyl ethanone	$C_8H_{14}O$		823-76-7
20	cyclohexyl ethanoate	$C_8H_{14}O_2$		622-45-7
21	cyclohexyl ether	$C_{12}H_{22}O$		4645-15-2
22	cyclohexyl hexanoate	$C_{12}H_{22}O_2$		6243-10-3
23	cyclohexyl pentanoate	$C_{11}H_{20}O_2$		1551-43-5
24	2-cyclohexylidencyclohexanone	$C_{12}H_{18}O$		1011-12-7
25	cyclopentanol	$C_5H_{10}O$		96-41-3
26	cyclopentanone	C_7H_8O		120-92-3
27	3,3-dimethylhexane	C_8H_{18}		563-16-6

No.	Compound	Formula	Chemical Structure	CAS#
28	4-(1,1-dimethylpropyl)cyclohexanone	$C_{11}H_{20}O$		16587-71-6
29	2-ethylidenecyclohexanone	$C_8H_{12}O$		1122-25-4
30	formic acid	CH_2O_2		64-18-6
31	2-heptanone	$C_7H_{14}O$		110-43-0
32	3-heptanone	$C_7H_{14}O$		106-35-4
33	hexanal	$C_6H_{12}O$		66-25-1
34	2-hexanone	$C_6H_{12}O$		591-78-6
35	5-hexenal	$C_6H_{10}O$		764-59-0
36	1-methoxycyclohexane	$C_7H_{14}O$		931-56-6
37	5-methyl-2-isopropylidenecyclohexanone	$C_{10}H_{16}O$		15932-80-6
38	2-methyl-3-heptanone	$C_8H_{16}O$		13019-20-0
39	methylcyclohexane	C_7H_{14}		108-87-2

No.	Compound	Formula	Chemical Structure	CAS#
40	2-methylcyclohexanone	$C_7H_{12}O$		583-60-8
41	3-methylcyclohexanone	$C_7H_{12}O$		591-24-2
42	methylcyclopentane	C_6H_{12}		96-37-7
43	1-methylcyclopentanol	$C_6H_{12}O$		1462-03-9
44	(1-methylethyl)cyclohexane	C_9H_{18}		696-29-7
45	2-methylcyclopentanone	$C_6H_{10}O$		1120-72-5
46	1-pentanol	$C_5H_{12}O$		71-41-0
47	2-pentanone	$C_5H_{10}O$		107-87-9
48	3-pentyl-1-cyclohexene	$C_{11}H_{20}$		15232-92-5
49	pentylcyclohexane	$C_{11}H_{22}$		4292-92-6
50	phenol	C_6H_6O		108-95-2
51	p-tert-butylcyclohexanol	$C_{10}H_{20}O$		98-52-2

No.	Compound	Formula	Chemical Structure	CAS#
52	2-tetrahydrofurylmethanol	$C_5H_{10}O_2$		97-99-4
53	1,2,3,4-tetrahydronaphthalene	$C_{10}H_{12}$		119-64-2
54	toluene	C_7H_8		108-88-3

Appendix C. Mathematics of the Joback Method

Equations used to estimate the thermophysical properties of pure substances by the Joback method are compiled in Table A1. The estimated values for the selected compounds in this work are shown in Table A2.

Table A1. Parameters and equations used in the Joback method.

Property	Parameter	Equation
Boiling temperature/K	$\tau_{b,k}$	$T_b^o = 198.2 + \sum_k N_k \tau_{b,k}$
Melting temperature/K	$\tau_{f,k}$	$T_m^o = 122.5 + \sum_k N_k \tau_{f,k}$
Critical temperature/K	$\tau_{c,k}$	$T_c = T_b \left[0.584 + 0.965 \sum_k N_k \tau_{c,k} - \left(\sum_k N_k \tau_{c,k} \right)^2 \right]^{-1}$
Critical pressure/bar	$\pi_{c,k}$	$p_c = \left(0.113 + 0.0032 N_{atoms} - \sum_k N_k \pi_{c,k} \right)^{-2}$
Critical volume/cm^3·mol^{-1}	$v_{c,k}$	$v_c = 17.5 + \sum_k N_k v_{c,k}$
Gibbs energy of formation/kJ·kmol^{-1}	$\Delta g_{f,k}$	$\Delta g_f^o = 53.88 + \sum_k N_k \Delta g_{f,k}$
Enthalpy of formation/kJ·kmol^{-1}	$\Delta h_{f,k}$	$\Delta h_f^o = 68.29 + \sum_k N_k \Delta h_{f,k}$
Enthalpy of vaporization/kJ·kmol^{-1}	$\Delta h_{v,k}$	$\Delta h_v^o = 15.3 + \sum_k N_k \Delta h_{v,k}$
Enthalpy of melting/kJ·kmol^{-1}	$\Delta h_{m,k}$	$\Delta h_m^o = -0.88 + \sum_k N_k \Delta h_{m,k}$
Isobaric thermal capacity/kJ·kmol^{-1}·K^{-1}	$c_{p,k}^A$; $c_{p,k}^B$ $c_{p,k}^C$; $c_{p,k}^D$	$c_p^o = \sum_k N_k c_{p,k}^A - 37.93 + T \left(\sum_k N_k c_{p,k}^B + 0.210 \right) +$ $+ T^2 \left(\sum_k N_k c_{p,k}^C - 3.91 \cdot 10^{-4} \right) + T^3 \left(\sum_k N_k c_{p,k}^D + 2.06 \cdot 10^{-7} \right)$

where N_k is the number of groups of type "k" in the molecule whose properties are to be calculated and N_{atoms} is the total number of atoms in it. The parameters $\tau_{b,k}$, $\tau_{f,k}$, $\tau_{c,k}$, and are the group contributions for the boiling, melting, and critical temperatures, respectively; $\pi_{c,k}$ is the contribution parameter for the critical pressure, $v_{c,k}$ is that of the critical volume, $\Delta g_{f,k}$ is the group contribution parameter for the Gibbs energy of formation, and $\Delta h_{f,k}$, $\Delta h_{v,k}$, $\Delta h_{m,k}$ are those corresponding to the enthalpies of formation, vaporization and melting, respectively; $c_{p,k}^A$; $c_{p,k}^B$; $c_{p,k}^C$; $c_{p,k}^D$ are the group contributions to calculate the thermal capacities.

Table A2. Properties estimated by the Joback method [14] for the selected compounds in this work.

No.	Compound	T_b^o K	T_m^o K	T_c K	p_c bar	v_c m^3/kmol	Δh_f^o kJ/mol	Δg_f^o kJ/mol	Δh_v^o kJ/mol	Δh_m^o kJ/mol	c_p (298 K) J/(molK)
1	acetic acid	390.7	272.9	587.3	57.31	0.171	−434.8	−377.9	40.67	11.08	65.7
2	1,1′-bicyclohexyl	544.3	262.8	782.6	27.35	0.587	−320.5	0.8	47.85	16.39	275.0
3	[1,1′-bicyclohexyl]-2,3′-dione	648.7	376.2	909.1	27.99	0.588	−457.8	−146.1	63.11	9.53	219.2
4	1-butanol	406.7	190.1	571.1	39.76	0.344	−354.6	−198.0	43.25	12.87	138.0
5	butoxycyclohexane	470.2	232.1	665.9	25.25	0.547	−327.6	−47.2	40.69	14.68	238.0
6	butylcyclohexane	447.8	209.8	644.6	25.69	0.529	−195.4	57.8	38.28	13.49	223.0
7	2-butylcyclohexanone	515.6	278.1	729.1	26.63	0.536	−333.1	−64.8	42.53	13.00	228.0
8	cycloheptanone	455.9	245	689.2	39.46	0.361	−257.0	−94.5	36.33	2.06	123.0
9	1,2-cyclohexanediol	502.8	358.9	720.4	34.8	0.342	−464.9	−273.6	53.77	16.55	195.0

Table A2. *Cont.*

No.	Compound	T_b^o K	T_m^o K	T_c K	p_c bar	v_c m^3/kmol	Δh_f^o kJ/mol	Δg_f^o kJ/mol	Δh_v^o kJ/mol	Δh_m^o kJ/mol	c_p (298 K) J/(molK)
10	1,3-cyclohexanedione	496.5	305.4	743.3	45.29	0.319	−367.9	−213.3	48.19	1.08	114.7
11	cyclohexanol	431.9	264	654.6	49.25	0.270	−278.7	−120.9	41.73	9.30	147.0
12	cyclohexanone	428.7	237.2	656.0	43.23	0.313	−230.2	−90.8	33.94	1.57	105.0
13	2-cyclohexen-1-ol	431.0	264.7	656.2	62.89	0.257	−220.9	−90.9	42.02	10.53	140.0
14	2-cyclohexen-1-one	427.9	238	654.8	45.35	0.299	−172.4	−60.8	34.23	2.79	97.5
15	1-(1-cyclohexen-1-yl)-2-propanone	488.6	271.8	707.4	34.04	0.458	−180.8	12.0	43.46	14.40	190.0
16	cyclohexene	360.1	169.8	566.9	43.28	0.292	−34.7	61.8	29.98	3.28	92.6
17	cyclohexylacetone	478.7	248.5	689.0	30.39	0.479	−287.4	−79.6	42.80	12.50	201.0
18	cyclohexyl butanoate	506.0	252.2	708.4	25.82	0.555	−512.7	−252.6	45.69	17.86	239.0
19	cyclohexylethanone	455.9	237.2	669.2	33.88	0.423	−266.7	−88.0	40.58	9.91	178.0
20	cyclohexyl ethanoate	460.2	229.1	668.4	41.52	0.443	−471.4	−269.4	40.94	14.44	169.0
21	cyclohexyl ether	544.3	262.8	782.6	26.46	0.587	−320.5	0.8	47.85	16.39	275.0
22	cyclohexyl hexanoate	551.7	274.7	748.6	21.43	0.667	−554.0	−235.8	50.14	23.04	285.0
23	cyclohexyl pentanoate	528.9	263.4	728.5	23.47	0.611	−533.3	−244.2	47.92	20.45	262.0
24	2-cyclohexylidencyclohexanone	621.1	362.1	872.0	27.33	0.606	−235.8	43.5	59.44	11.56	220.1
25	cyclopentanol	404.7	256.2	621.0	54.55	0.223	−251.9	−117.2	39.33	8.81	129.0
26	cyclopentanone	401.6	229.5	622.3	47.56	0.265	−203.4	−87.1	31.54	1.08	87.0
27	3,3-dimethylhexane	379.2	182.3	553.4	25.85	0.473	−217.2	19.3	34.77	14.67	184.0
28	4-(1,1-dimethylpropyl)cyclohexanone	535.2	291.8	758.9	24.63	0.581	−362.5	−53.6	46.13	13.79	251.0
29	2-ethylidenecyclohexanone	481.1	270.1	709.8	35.26	0.408	−195.5	−28.5	39.62	7.07	142.0
30	formic acid	363.1	203.8	534.4	75.88	0.127	−301.8	−278.6	43.65	4.72	46.1
31	2-heptanone	413.4	218.58	590.0	29.96	0.434	−300.4	−120.9	39.08	15.49	167.3
32	3-heptanone	413.4	218.58	590.0	29.96	0.434	−300.4	−120.9	39.08	15.49	167.3
33	hexanal	385.3	198.9	557.8	36.47	0.389	−252.8	−99.9	35.37	15.35	148.0
34	2-hexanone	390.6	206.8	568.1	35.99	0.378	−279.8	−129.3	35.30	14.66	144.0
35	5-hexenal	382.0	197.1	558.1	35.52	0.370	−127.3	−12.0	34.70	14.07	137.0
36	1-Methoxycyclohexane	374.4	190.5	569.6	33.53	0.331	−238.9	−68.8	31.62	6.42	151.0
37	5-methyl-2-isopropylidenecyclohexanone	522.1	274.5	755.1	27.58	0.520	−266.9	−27.9	43.40	12.01	219.0
38	2-methyl-3-heptanone	435.8	214.8	615.2	27.27	0.483	−326.3	−114.8	40.96	14.55	189.2
39	Methylcyclohexane	379.1	176	581.6	35.22	0.361	−133.5	32.5	31.61	5.72	155.0
40	2-methylcyclohexanone	352.0	168.28	546.9	38.39	0.313	−106.7	36.2	29.40	5.23	112.6
41	3-methylcyclohexanone	352.0	168.28	546.9	38.39	0.313	−106.7	36.2	29.40	5.23	112.6
42	1-methylcyclopentanol	427.8	291.4	651.6	50.66	0.277	−257.3	−114.3	40.41	5.11	121.0
43	2-methylcyclopentanone	419.8	236.5	637.4	40.11	0.320	−244.4	−86.4	37.61	4.74	117.5
44	(1-methylethyl)cyclohexane	424.4	183.6	628.2	28.63	0.467	−180.1	46.9	35.67	7.38	200.0
45	methylcyclopentanone	351.9	168.2	546.9	38.39	0.312	−106.6	36.1	29.40	5.23	111.7
46	1-pentanol	406.0	206.9	567.6	38.77	0.335	−298.8	−145.6	43.40	12.79	131.0
47	2-pentanone	367.6	196	545.9	37.41	0.321	−259.1	−137.7	33.96	10.30	120.7
48	3-pentyl-1-cyclohexene	469.8	221.9	666.3	24.19	0.571	−158.3	96.2	40.80	17.30	239.0
49	pentylcyclohexane	470.6	221.1	665.2	23.36	0.585	−216.1	66.2	40.51	16.08	246.0
50	phenol	439.0	283	671.0	59.26	0.230	−96.5	−32.9	43.58	11.51	95.2
51	p-tert-butylcyclohexanol	523.6	271.8	729.8	25.77	0.576	−270.8	−32.7	50.04	18.90	214.3
52	2-tetrahydrofurylmethanol	449.3	235.8	635.2	48.29	0.315	−399.6	−227.7	48.45	14.06	125.0
53	1,2,3,4-tetrahydronaphthalene	475.5	260.1	708.1	35.69	0.438	62.3	192.5	41.19	10.27	144.0
54	toluene	386.2	195.1	597.8	41.14	0.320	48.7	120.5	33.45	7.93	102.0

Appendix D. Mathematics of the Marrero–Gani Method

The Marrero–Gani method estimates the same properties as the Joback method, with the exception of the thermal capacity. The combination of groups of different order is performed in the same way for each property, following Equation (A1):

$$f = \sum_{i} N_i A_i^1 + \sum_{j} M_j A_j^2 + \sum_{k} O_k A_k^3 \tag{A1}$$

where N_i, M_j, and O_k are, respectively, the number groups of first, second, or third order for a given type present in the molecule, and A_i^1, A_j^2, and A_k^3 are the characteristic parameters of the corresponding group. The function f varies according to the property to be estimated, as shown in Table A3. The constants used for that function are presented in Table A4. Results obtained from the application of the method for the selected compounds are shown in Table A5.

Table A3. Equations used in the Marrero–Gani method [15] for estimating the different thermophysical properties.

Property	f=	Right-Hand Side of Equation (A1)
Melting temperature/K	$\exp(T_m^o/T_{m,0}^o)$	$\sum_i N_i T_{m1i}^o + \sum_j M_j T_{m2j}^o + \sum_k O_k T_{m3k}^o$
Boiling temperature/K	$\exp(T_b^o/T_{b,0}^o)$	$\sum_i N_i T_{b1i}^o + \sum_j M_j T_{b2j}^o + \sum_k O_k T_{b3k}^o$

Table A3. *Cont.*

Property	f=	Right-Hand Side of Equation (A1)
Critical temperature/K	$\exp(T_c/T_{c0})$	$\sum_i N_i T_{c1i} + \sum_j M_j T_{c2j} + \sum_k O_k T_{c3k}$
Critical pressure/bar	$(p_c - p_{c1})^{-0.5} - p_{c2}$	$\sum_i N_i p_{c1i} + \sum_j M_j p_{c2j} + \sum_k O_k p_{c3k}$
Critical volume/cm^3·mol^{-1}	$v_c - v_{c0}$	$\sum_i N_i v_{c1i} + \sum_j M_j v_{c2j} + \sum_k O_k v_{c3k}$
Gibbs energy of formation/kJ·kmol^{-1}	$\Delta g_f^o - \Delta g_{f,0}^o$	$\sum_i N_i g_{f1i}^o + \sum_j M_j g_{f2j}^o + \sum_k O_k g_{f3k}^o$
Enthalpy of formation/kJ·kmol^{-1}	$\Delta h_f^o - \Delta h_{f,0}^o$	$\sum_i N_i h_{f1i}^o + \sum_j M_j h_{f2j}^o + \sum_k O_k h_{f3k}^o$
Enthalpy of vaporization/kJ·kmol^{-1}	$\Delta h_v^o - \Delta h_{v,0}^o$	$\sum_i N_i h_{v1i}^o + \sum_j M_j h_{v2j}^o + \sum_k O_k h_{v3k}^o$
Enthalpy of melting/kJ·kmol^{-1}	$\Delta h_m^o - \Delta h_{m,0}^o$	$\sum_i N_i h_{m1i}^o + \sum_j M_j h_{m2j}^o + \sum_k O_k h_{m3k}^o$

Table A4. Generic constants used in the Marrero–Gani method [15] for equations shown in Table A3.

Generic Constants	
$T_{m,0}^o$/K	147.450
$T_{b,0}^o$/K	222.543
T_{c0}/K	231.239
p_{c1}/bar	5.9827
p_{c2}/bar$^{-0.5}$	0.108998
$v_{c0/}$cm^3·mol^{-1}	7.95
$\Delta g_{f,0}^o$/kJ·mol^{-1}	−34.967
$\Delta h_{f,0}^o$/kJ·mol^{-1}	5.549
$\Delta h_{v,0}^o$/kJ·mol^{-1}	11.733
$\Delta h_{m,0}^o$/kJ·mol^{-1}	−2.806

Table A5. Properties estimated by the Marrero–Gani method [15] for the selected compounds used in this work.

No.	Compound	T_b^o K	T_m^o K	T_c K	p_c bar	v_c m^3/kmol	Δg_f^o kJ/mol	Δh_f^o kJ/mol	Δh_v^o kJ/mol	Δh_m^o kJ/mol
1	acetic acid	397.3	308.4	646.20	58.88	0.159	−369.2	−426.9	28.95	9.55
2	1,1′-bicyclohexyl	511.7	271.7	727.00	25.60	0.598	42.6	−272.0	57.98	12.91
3	[1,1′-bicyclohexyl]-2,3′-dione	579.8	354.2	867.22	30.29	0.599	−528.3	−229.8	85.54	23.04
4	1-butanol	381.7	213.0	553.80	43.70	0.276	−277.8	−151.9	50.83	10.93
5	Butoxycyclohexane	464.5	231.5	676.94	22.89	0.610	−40.9	−357.0	59.80	19.52
6	butylcyclohexane	454.1	199.4	650.20	25.40	0.533	70.0	−200.3	49.37	13.49
7	2-Butylcyclohexanone	493.3	286.4	762.27	27.58	0.544	−105.3	−366.3	63.58	19.70
8	cycloheptanone	451.7	278.9	734.20	41.37	0.361	−111.9	−286.1	48.90	9.75
9	1,2-cyclohexanediol	504.2	349.0	714.14	44.00	0.341	−263.8	−466.5	90.63	16.06
10	1,3-cyclohexanedione	493.4	331.6	807.20	51.56	0.312	−295.2	−429.1	58.73	13.74
11	cyclohexanol	434.0	287.8	650.00	42.60	0.322	−109.5	−286.2	61.20	9.84
12	cyclohexanone	431.2	265.7	715.26	45.93	0.312	−125.2	−267.5	45.56	8.68
13	2-cyclohexen-1-ol	437.2	288.9	648.32	45.39	0.307	−49.6	−189.2	62.29	8.88
14	2-cyclohexen-1-one	443.2	267.8	714.00	49.12	0.297	−59.2	−183.0	53.06	10.23
15	1-(1-cyclohexen-1-yl)-2-propanone	470.7	262.3	685.83	31.52	0.460	−27.4	−205.9	52.37	14.73
16	cyclohexene	356.1	183.6	558.00	43.92	0.289	104.7	−8.9	32.86	2.66
17	cyclohexylacetone	473.7	266.4	679.01	29.83	0.483	−75.0	−301.2	54.96	15.75
18	cyclohexyl butanoate	486.2	237.2	683.41	25.83	0.545	−245.5	−543.1	61.08	18.83
19	cyclohexylethanone	453.7	278.5	662.05	33.33	0.427	−83.1	−280.4	49.43	13.11
20	cyclohexyl ethanoate	441.0	225.4	639.90	31.20	0.448	−481.9	−267.1	53.53	12.88
21	cyclohexyl ether	515.7	281.6	732.56	26.16	0.608	−3.9	−342.5	64.85	16.71
22	cyclohexyl hexanoate	515.7	257.9	727.13	20.21	0.713	−221.3	−605.5	75.81	26.75
23	cyclohexyl pentanoate	497.7	244.4	698.92	23.63	0.601	−237.4	−563.9	65.99	21.47
24	2-cyclohexylidencyclohexanone	565.4	323.2	783.20	31.56	0.501	−72.1	−341.8	58.93	12.95
25	cyclopentanol	413.4	275.3	622.23	47.41	0.273	−122.8	−267.6	57.86	11.73
26	cyclopentanone	403.8	251.1	694.64	51.44	0.262	−138.5	−248.9	42.22	7.61
27	3,3-dimethylhexane	385.1	187.3	555.14	25.68	0.466	17.2	−217.9	38.06	10.52
28	4-(1,1-dimethylpropyl)cyclohexanone	503.9	298.3	776.91	27.06	0.575	−90.3	−392.6	65.55	16.86
29	2-ethylidenecyclohexanone	478.4	276.7	737.22	33.74	0.448	−47.1	−211.7	63.55	11.38
30	formic acid	362.8	259.4	554.90	83.20	0.102	−279.9	−303.6	48.32	13.31
31	2-heptanone	426.7	223.8	611.13	29.34	0.417	−300.8	−122.0	46.38	17.58
32	3-heptanone	417.1	227.2	596.91	29.44	0.418	−305.0	−125.4	46.29	17.26
33	hexanal	407.6	228.8	591.00	33.10	0.373	−251.1	−100.7	43.90	20.10
34	2-hexanone	400.8	215.1	589.20	32.47	0.373	−278.6	−127.6	41.82	14.20
35	5-hexenal	405.6	232.5	594.10	34.76	0.359	−128.8	−14.9	42.80	17.07
36	1-Methoxycyclohexane	408.2	203.4	607.23	32.33	0.406	−63.2	−279.8	37.51	10.73

Table A5. *Cont.*

No.	Compound	T_b^o K	T_m^o K	T_c K	p_c bar	v_c m^3/kmol	Δg_f^o kJ/mol	Δh_f^o kJ/mol	Δh_v^o kJ/mol	Δh_m^o kJ/mol
37	5-methyl-2-isopropylidenecyclohexanone	497.2	299.0	753.09	28.05	0.558	−33.8	−255.2	77.19	11.98
38	2-methyl-3-heptanone	431.2	233.0	613.20	26.78	0.470	−122.8	−334.2	49.16	16.81
39	Methylcyclohexane	374.2	182.4	577.23	35.07	0.370	44.6	−137.8	35.17	6.74
40	2-methylcyclohexanone	448.3	266.3	723.99	38.52	0.370	−299.4	−125.3	48.95	11.81
41	3-methylcyclohexanone	448.3	266.3	723.99	38.52	0.370	−299.4	−125.3	48.95	11.81
42	1-methylcyclopentanol	409.2	283.5	580.05	44.29	0.325	−142.0	−313.4	57.35	5.99
43	2-methylcyclopentanone	422.4	251.8	704.16	42.52	0.321	−280.8	−138.6	45.61	10.74
44	(1-methylethyl)cyclohexane	427.9	191.4	621.05	28.42	0.481	57.3	−196.4	43.00	11.32
45	methylcyclopentanone	340.4	155.8	538.30	38.44	0.313	31.3	−119.2	31.83	5.64
46	1-pentanol	410.9	221.5	580.32	38.12	0.332	−143.9	−298.6	55.80	14.20
47	2-pentanone	362.1	210.4	544.80	37.06	0.306	−141.6	−263.3	36.47	11.98
48	3-pentyl-1-cyclohexene	473.2	180.7	652.99	25.51	0.559	128.8	−109.7	59.95	16.49
49	pentylcyclohexane	476.9	208.7	668.01	23.27	0.590	78.0	−221.2	54.28	16.13
50	phenol	455.0	308.0	687.06	59.65	0.271	−32.6	−94.3	64.25	15.36
51	p-tert-butylcyclohexanol	494.8	240.6	694.60	24.12	0.595	216.4	−43.5	58.23	13.72
52	2-tetrahydrofurylmethanol	451.2	258.3	641.69	48.15	0.305	−239.0	−399.2	64.17	14.14
53	1,2,3,4-tetrahydronaphthalene	480.8	241.7	664.03	31.37	0.521	110.1	−61.3	77.10	11.86
54	toluene	383.8	202.1	604.05	42.18	0.317	123.6	50.6	38.43	9.90

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