

SUPPORTING INFORMATION

Chapter 2.2: Detailed results for vapor pressure estimation of esters and acids.

Tables 1-8 show detailed results for vapor pressure estimations for each model. As for the saturated acids, deviations partly show a tendency to increase with increasing chain length. In case of C18:0 (methyl stearate), considerable deviations are found in regions I, II and IV using the models of Moller / Rarey / Ramjugernath, Nannoolal / Rarey / Ramjugernath (given T_b), Gomez-Nieto / Thodos and Riedel; these models use T_b as user input. On the other hand, Nannoolal / Rarey / Ramjugernath (estimated T_b), Ambrose / Walton and Lee / Kesler show moderate deviations for this substance, using molecular structure (Nannoolal / Rarey / Ramjugernath) or critical temperature with acentric factor (Ambrose / Walton and Lee / Kesler) for estimation. This indicates that the measured normal boiling point temperature is questionable.

The four above mentioned models which use the normal boiling point as user input yield considerable deviations in the low pressure regions I and II in case of C20:0 (methyl eicosanoate) and C22:0 (methyl docosanoate), while the normal boiling point is estimated properly; this indicates that the low pressure data are questionable.

Table 1. Results (RMD) for vapor pressure estimation of esters and acids with the Moller / Rarey / Ramjugernath group contribution model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	12.3 ⁵²	6.0 ²⁴	5.7 ⁹	-	8.6 ²	9.8 ⁸⁷
C14:0	methyl myristate	8.2 ⁵³	4.9 ²⁴	1.9 ⁸	-	1.9 ¹	6.6 ⁸⁶
C16:0	methyl palmitate	23.4 ⁷⁰	8.3 ³⁰	-	1.7 ¹	-	18.7 ¹⁰¹
C18:0	methyl stearate	73.4 ⁶⁵	39.4 ²⁵	-	19.8 ¹	-	63.5 ⁹¹
C18:1	methyl oleate	20.4 ²⁸	10.7 ¹¹	-	-	4.8 ¹	17.3 ⁴⁰
C18:2	methyl linoleate	6.9 ¹⁸	14.9 ⁶	-	-	0.0 ¹	8.5 ²⁵
C18:3	methyl linolenate	7.4 ⁹	-	-	-	0.0 ¹	6.7 ¹⁰
C20:0	methyl arachidate	28.8 ¹⁷	25.9 ¹	-	-	0.0 ¹	27.2 ¹⁹

C22:0	methyl behenate	92.2 ¹⁷	23.5 ¹	-	-	0.0 ¹	83.7 ¹⁹
C12:0	lauric acid	9.4 ³⁵	11.5 ⁶⁹	7.0 ⁵	1.4 ¹	0.7 ¹	10.4 ¹¹¹
C14:0	myristic acid	23.0 ⁵⁰	17.9 ⁵²	10.5 ³	2.3 ¹	-	20.0 ¹⁰⁶
C16:0	palmitic acid	39.8 ³³	25.6 ⁹	17.1 ⁴	-	-	35.1 ⁴⁶
C18:0	stearic acid	56.0 ³¹	31.4 ⁶	20.5 ⁴	-	-	48.9 ⁴¹
C18:1	oleic acid	53.8 ²⁰	20.0 ⁸	2.8 ⁴	13.4 ¹	16.5 ³	36.4 ³⁶
average		32.5 ⁴⁹⁸	18.4 ²⁶⁶	9.4 ³⁷	7.7 ⁵	3.6 ¹²	28.1 ⁸¹⁸

Table 2. Results (RMD) for vapor pressure estimation of esters and acids with the Nannoolal / Rarey / Ramjugernath / with given T_b group contribution model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	6.2 ⁵²	6.9 ²⁴	7.1 ⁹	-	8.7 ²	6.5 ⁸⁷
C14:0	methyl myristate	20.4 ⁵³	4.7 ²⁴	1.5 ⁸	-	1.9 ¹	14.0 ⁸⁶
C16:0	methyl palmitate	57.4 ⁷⁰	6.7 ³⁰	-	1.7 ¹	-	41.8 ¹⁰¹
C18:0	methyl stearate	101.2 ⁶⁵	34.1 ²⁵	-	20.2 ¹	-	81.9 ⁹¹
C18:1	methyl oleate	19.8 ²⁸	7.0 ¹¹	-	-	4.9 ¹	15.9 ⁴⁰
C18:2	methyl linoleate	8.6 ¹⁸	14.6 ⁶	-	-	0.0 ¹	9.7 ²⁵
C18:3	methyl linolenate	13.0 ⁹	-	-	-	0.0 ¹	11.7 ¹⁰
C20:0	methyl arachidate	97.8 ¹⁷	20.7 ¹	-	-	0.0 ¹	88.6 ¹⁹
C22:0	methyl behenate	91.6 ¹⁷	17.2 ¹	-	-	0.0 ¹	82.9 ¹⁹
C12:0	lauric acid	60.8 ³⁵	9.6 ⁶⁹	10.0 ⁵	3.0 ¹	0.7 ¹	25.6 ¹¹¹
C14:0	myristic acid	37.1 ⁵⁰	18.3 ⁵²	15.0 ³	4.5 ¹	-	26.9 ¹⁰⁶
C16:0	palmitic acid	42.3 ³³	26.7 ⁹	22.1 ⁴	-	-	37.5 ⁴⁶
C18:0	stearic acid	26.9 ³¹	32.6 ⁶	25.5 ⁴	-	-	27.6 ⁴¹
C18:1	oleic acid	28.6 ²⁰	23.9 ⁸	8.0 ⁴	18.0 ¹	21.3 ³	24.3 ³⁶
average		43.7 ⁴⁹⁸	17.2 ²⁶⁶	12.8 ³⁷	9.5 ⁵	4.2 ¹²	35.4 ⁸¹⁸

Table 3. Results (RMD) for vapor pressure estimation of esters and acids with the Nannoolal / Rarey / Ramjugernath / with estimated T_b group contribution model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	8.4 ⁵²	3.3 ²⁴	1.9 ⁹	-	4.4 ²	6.2 ⁸⁷
C14:0	methyl myristate	21.8 ⁵³	4.7 ²⁴	1.2 ⁸	-	2.7 ¹	14.9 ⁸⁶
C16:0	methyl palmitate	47.7 ⁷⁰	5.3 ³⁰	-	1.4 ¹	-	34.7 ¹⁰¹

C18:0	methyl stearate	31.8 ⁶⁵	4.1 ²⁵	-	3.6 ¹	-	23.9 ⁹¹
C18:1	methyl oleate	16.3 ²⁸	9.5 ¹¹	-	-	6.6 ¹	14.2 ⁴⁰
C18:2	methyl linoleate	8.9 ¹⁸	13.4 ⁶	-	-	5.9 ¹	9.9 ²⁵
C18:3	methyl linolenate	9.8 ⁹	-	-	-	1.7 ¹	9.0 ¹⁰
C20:0	methyl arachidate	58.8 ¹⁷	6.4 ¹	-	-	8.7 ¹	53.4 ¹⁹
C22:0	methyl behenate	90.2 ¹⁷	7.4 ¹	-	-	6.3 ¹	81.4 ¹⁹
C12:0	lauric acid	27.3 ³⁵	33.0 ⁶⁹	30.8 ⁵	23.2 ¹	19.5 ¹	30.9 ¹¹¹
C14:0	myristic acid	27.7 ⁵⁰	39.8 ⁵²	34.7 ³	24.6 ¹	-	33.8 ¹⁰⁶
C16:0	palmitic acid	26.6 ³³	47.6 ⁹	41.9 ⁴	-	-	32.0 ⁴⁶
C18:0	stearic acid	32.1 ³¹	51.5 ⁶	44.3 ⁴	-	-	36.2 ⁴¹
C18:1	oleic acid	66.5 ²⁰	66.0 ⁸	55.1 ⁴	57.9 ¹	45.1 ³	63.1 ³⁶
average		33.8 ⁴⁹⁸	22.5 ²⁶⁶	30.0 ³⁷	22.2 ⁵	11.2 ¹²	31.7 ⁸¹⁸

Table 4. Results (RMD) for vapor pressure estimation of esters and acids with the Ceriani (2013) biodiesel-specific group contribution model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	14.9 ⁵²	4.5 ²⁴	1.4 ⁹	-	4.8 ²	10.4 ⁸⁷
C14:0	methyl myristate	19.1 ⁵³	5.7 ²⁴	1.7 ⁸	-	2.3 ¹	13.5 ⁸⁶
C16:0	methyl palmitate	26.0 ⁷⁰	8.6 ³⁰	-	0.0 ¹	-	20.5 ¹⁰¹
C18:0	methyl stearate	28.3 ⁶⁵	9.8 ²⁵	-	1.1 ¹	-	22.9 ⁹¹
C18:1	methyl oleate	21.7 ²⁸	8.1 ¹¹	-	-	4.8 ¹	17.5 ⁴⁰
C18:2	methyl linoleate	11.5 ¹⁸	15.1 ⁶	-	-	12.8 ¹	12.4 ²⁵
C18:3	methyl linolenate	20.9 ⁹	-	-	-	24.0 ¹	21.2 ¹⁰
C20:0	methyl arachidate	47.5 ¹⁷	1.9 ¹	-	-	0.3 ¹	42.7 ¹⁹
C22:0	methyl behenate	88.5 ¹⁷	9.8 ¹	-	-	9.9 ¹	80.2 ¹⁹
C12:0	lauric acid	13.1 ³⁵	4.1 ⁶⁹	2.3 ⁵	7.4 ¹	8.7 ¹	6.9 ¹¹¹
C14:0	myristic acid	6.9 ⁵⁰	3.5 ⁵²	5.5 ³	13.0 ¹	-	5.3 ¹⁰⁶
C16:0	palmitic acid	9.7 ³³	7.0 ⁹	6.2 ⁴	-	-	8.9 ⁴⁶
C18:0	stearic acid	18.0 ³¹	8.3 ⁶	8.2 ⁴	-	-	15.7 ⁴¹
C18:1	oleic acid	56.5 ²⁰	25.7 ⁸	3.5 ⁴	14.8 ¹	23.7 ³	39.9 ³⁶
average		27.3 ⁴⁹⁸	8.6 ²⁶⁶	4.1 ³⁷	7.3 ⁵	10.1 ¹²	22.7 ⁸¹⁸

Table 5. Results (RMD) for vapor pressure estimation of esters and acids with the Gomez-Nieto / Thodos corresponding-state model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa	10 kPa	40 kPa	> 100 kPa	overall

			to < 10 kPa	to < 40 kPa	to 100 kPa		
C12:0	methyl laurate	131.3 ⁵²	31.3 ²⁴	12.7 ⁹	-	8.0 ²	88.6 ⁸⁷
C14:0	methyl myristate	312.0 ⁵³	54.9 ²⁴	24.4 ⁸	-	1.8 ¹	209.9 ⁸⁶
C16:0	methyl palmitate	839.4 ⁷⁰	71.9 ³⁰	-	1.7 ¹	-	603.2 ¹⁰¹
C18:0	methyl stearate	1591.6 ⁶⁵	179.1 ²⁵	-	16.3 ¹	-	1186.2 ⁹¹
C18:1	methyl oleate	96.7 ²⁸	49.4 ¹¹	-	-	4.5 ¹	81.4 ⁴⁰
C18:2	methyl linoleate	162.5 ¹⁸	83.1 ⁶	-	-	0.0 ¹	136.9 ²⁵
C18:3	methyl linolenate	184.0 ⁹	-	-	-	0.0 ¹	165.6 ¹⁰
C20:0	methyl arachidate	2787.5 ¹⁷	154.8 ¹	-	-	0.0 ¹	2502.2 ¹⁹
C22:0	methyl behenate	113.0 ¹⁷	122.6 ¹	-	-	0.0 ¹	107.6 ¹⁹
C12:0	lauric acid	424.3 ³⁵	44.1 ⁶⁹	14.8 ⁵	2.5 ¹	0.6 ¹	161.9 ¹¹¹
C14:0	myristic acid	431.8 ⁵⁰	41.8 ⁵²	10.4 ³	1.9 ¹	-	224.5 ¹⁰⁶
C16:0	palmitic acid	776.5 ³³	38.4 ⁹	8.2 ⁴	-	-	565.3 ⁴⁶
C18:0	stearic acid	885.0 ³¹	33.8 ⁶	7.1 ⁴	-	-	674.8 ⁴¹
C18:1	oleic acid	2319.6 ²⁰	84.5 ⁸	48.0 ⁴	4.4 ¹	22.1 ³	1314.7 ³⁶
average		789.6 ⁴⁹⁸	76.1 ²⁶⁶	17.9 ³⁷	5.4 ⁵	4.1 ¹²	573.0 ⁸¹⁸

Table 6. Results (RMD) for vapor pressure estimation of esters and acids with the Riedel corresponding-state model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	42.2 ⁵²	14.4 ²⁴	6.3 ⁹	-	8.1 ²	30.0 ⁸⁷
C14:0	methyl myristate	138.6 ⁵³	36.6 ²⁴	18.4 ⁸	-	1.8 ¹	97.4 ⁸⁶
C16:0	methyl palmitate	381.0 ⁷⁰	52.8 ³⁰	-	1.7 ¹	-	279.7 ¹⁰¹
C18:0	methyl stearate	956.9 ⁶⁵	152.0 ²⁵	-	16.5 ¹	-	725.5 ⁹¹
C18:1	methyl oleate	36.1 ²⁸	22.7 ¹¹	-	-	4.5 ¹	31.6 ⁴⁰
C18:2	methyl linoleate	91.5 ¹⁸	56.8 ⁶	-	-	0.0 ¹	79.5 ²⁵
C18:3	methyl linolenate	95.0 ⁹	-	-	-	0.0 ¹	85.5 ¹⁰
C20:0	methyl arachidate	1157.9 ¹⁷	122.3 ¹	-	-	0.0 ¹	1042.5 ¹⁹
C22:0	methyl behenate	106.2 ¹⁷	96.8 ¹	-	-	0.0 ¹	100.1 ¹⁹
C12:0	lauric acid	188.5 ³⁵	23.1 ⁶⁹	7.8 ⁵	1.5 ¹	0.7 ¹	74.2 ¹¹¹
C14:0	myristic acid	184.3 ⁵⁰	20.7 ⁵²	4.6 ³	1.0 ¹	-	97.2 ¹⁰⁶
C16:0	palmitic acid	320.3 ³³	18.5 ⁹	3.7 ⁴	-	-	233.7 ⁴⁶
C18:0	stearic acid	338.8 ³¹	16.0 ⁶	2.4 ⁴	-	-	258.7 ⁴¹
C18:1	oleic acid	1254.5 ²⁰	67.2 ⁸	42.6 ⁴	2.9 ¹	22.3 ³	718.5 ³⁶
average		378.0 ⁴⁹⁸	53.9 ²⁶⁶	12.3 ³⁷	4.7 ⁵	4.2 ¹²	275.3 ⁸¹⁸

Table 7. Results (RMD) for vapor pressure estimation of esters and acids with the Ambrose / Walton corresponding-state model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	8.7 ⁵²	4.2 ²⁴	1.3 ⁹	-	12.3 ²	6.8 ⁸⁷
C14:0	methyl myristate	17.7 ⁵³	6.1 ²⁴	2.1 ⁸	-	8.9 ¹	12.9 ⁸⁶
C16:0	methyl palmitate	30.9 ⁷⁰	5.5 ³⁰	-	14.6 ¹	-	23.2 ¹⁰¹
C18:0	methyl stearate	19.7 ⁶⁵	3.8 ²⁵	-	17.0 ¹	-	15.3 ⁹¹
C18:1	methyl oleate	11.2 ²⁸	6.6 ¹¹	-	-	0.1 ¹	9.7 ⁴⁰
C18:2	methyl linoleate	65.1 ¹⁸	51.8 ⁶	-	-	34.0 ¹	60.7 ²⁵
C18:3	methyl linolenate	19.8 ⁹	-	-	-	9.6 ¹	18.7 ¹⁰
C20:0	methyl arachidate	114.6 ¹⁷	33.1 ¹	-	-	16.6 ¹	105.1 ¹⁹
C22:0	methyl behenate	91.4 ¹⁷	23.8 ¹	-	-	29.2 ¹	84.5 ¹⁹
C12:0	lauric acid	62.0 ³⁵	4.1 ⁶⁹	8.4 ⁵	9.3 ¹	8.8 ¹	22.6 ¹¹¹
C14:0	myristic acid	50.4 ⁵⁰	6.8 ⁵²	11.6 ³	10.2 ¹	-	27.5 ¹⁰⁶
C16:0	palmitic acid	60.7 ³³	15.8 ⁹	18.8 ⁴	-	-	48.3 ⁴⁶
C18:0	stearic acid	60.2 ³¹	16.9 ⁶	18.7 ⁴	-	-	49.8 ⁴¹
C18:1	oleic acid	164.8 ²⁰	18.8 ⁸	4.8 ⁴	24.8 ¹	35.8 ³	99.9 ³⁶
average		55.5 ⁴⁹⁸	15.2 ²⁶⁶	9.4 ³⁷	15.2 ⁵	17.3 ¹²	41.8 ⁸¹⁸

Table 8. Results (RMD) for vapor pressure estimation of esters and acids with the Lee / Kesler corresponding-state model. The number in superscript specifies the number of data points used.

pressure region		I	II	III	IV	V	
component		< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
C12:0	methyl laurate	9.2 ⁵²	3.5 ²⁴	2.0 ⁹	-	11.7 ²	6.9 ⁸⁷
C14:0	methyl myristate	20.6 ⁵³	5.1 ²⁴	2.5 ⁸	-	8.2 ¹	14.5 ⁸⁶
C16:0	methyl palmitate	40.7 ⁷⁰	5.7 ³⁰	-	13.9 ¹	-	30.0 ¹⁰¹
C18:0	methyl stearate	26.8 ⁶⁵	3.8 ²⁵	-	16.4 ¹	-	20.4 ⁹¹
C18:1	methyl oleate	11.3 ²⁸	6.2 ¹¹	-	-	1.0 ¹	9.6 ⁴⁰
C18:2	methyl linoleate	64.1 ¹⁸	51.7 ⁶	-	-	33.6 ¹	59.9 ²⁵
C18:3	methyl linolenate	19.7 ⁹	-	-	-	8.8 ¹	18.6 ¹⁰
C20:0	methyl arachidate	148.9 ¹⁷	32.1 ¹	-	-	15.8 ¹	135.7 ¹⁹
C22:0	methyl behenate	91.2 ¹⁷	23.6 ¹	-	-	28.7 ¹	84.4 ¹⁹
C12:0	lauric acid	68.2 ³⁵	4.9 ⁶⁹	8.9 ⁵	9.0 ¹	8.3 ¹	25.1 ¹¹¹
C14:0	myristic acid	57.5 ⁵⁰	7.6 ⁵²	11.7 ³	9.8 ¹	-	31.3 ¹⁰⁶
C16:0	palmitic acid	75.1 ³³	16.2 ⁹	18.9 ⁴	-	-	58.7 ⁴⁶
C18:0	stearic acid	78.3 ³¹	17.1 ⁶	18.7 ⁴	-	-	63.6 ⁴¹
C18:1	oleic acid	185.3 ²⁰	18.6 ⁸	4.7 ⁴	24.5 ¹	35.3 ³	111.2 ³⁶

average	64.1 ⁴⁹⁸	15.1 ²⁶⁶	9.6 ³⁷	14.7 ⁵	16.8 ¹²	47.8 ⁸¹⁸
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Chapter 3.1: Detailed results for vapor pressure estimation of triglycerides using original

T_b from the data banks

Tables 9-12 show detailed results for vapor pressure estimations for each model.

Table 9. Results for vapor pressure estimation (RMD) of triglycerides with Moller / Rarey / Ramjugernath model, using original normal boiling points. The number in superscript is the number of data points used. The two substances –CH₂– 18 and 24 were excluded from average.

pressure region	I	II	III	IV	V	
–CH ₂ –	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	2.5 ²	2.1 ⁵	0.9 ⁴	10.8 ⁶	5.0 ¹⁷
3	32.2 ²	37.5 ³	-	-	0.2 ¹	29.5 ⁶
6	33.9 ⁶	35.7 ⁴	11.3 ⁶	-	2.9 ²	23.3 ¹⁸
12	12.6 ⁶	22.5 ⁴	3.6 ³	16.3 ¹	6.5 ²	12.9 ¹⁶
15	98.2 ⁶	-	-	-	-	98.2 ⁶
(18)	(645.2 ⁸)	(112.5 ⁵)	(45.8 ³)	(17.9 ²)	(1.0 ²)	(294.9 ²⁰)
(24)	(3840.9 ⁶)	-	-	-	-	(3840.9 ⁶)
30	75.8 ⁶	-	-	-	-	75.8 ⁶
36	49.4 ⁶	-	-	-	-	49.4 ⁶
42	139.5 ⁶	-	-	-	-	139.5 ⁶
48	111.1 ⁶	-	-	-	-	111.1 ⁶
average	69.1 ⁴⁴	24.5 ¹³	5.7 ¹⁴	8.6 ⁵	5.1 ¹¹	60.5 ⁸⁷

Table 10. Results for vapor pressure estimation (RMD) of triglycerides with Nannoolal / Rarey / Ramjugernath / given T_b model, using original normal boiling points. The number in superscript is the number of data points used. The two substances –CH₂– 18 and 24 were excluded from average.

pressure region	I	II	III	IV	V	
–CH ₂ –	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	12.6 ²	8.3 ⁵	3.1 ⁴	12.5 ⁶	9.1 ¹⁷
3	42.5 ²	45.6 ³	-	-	0.2 ¹	37.0 ⁶
6	41.8 ⁶	43.7 ⁴	18.0 ⁶	-	3.0 ²	30.0 ¹⁸
12	10.2 ⁶	32.7 ⁴	9.3 ³	20.9 ¹	6.8 ²	15.9 ¹⁶
15	97.6 ⁶	-	-	-	-	97.6 ⁶

(18)	(460.8 ⁸)	(82.5 ⁵)	(40.3 ³)	(22.2 ²)	(1.1 ²)	(213.3 ²⁰)
(24)	(2535.2 ⁶)	-	-	-	-	(2535.2 ⁶)
30	32.0 ⁶	-	-	-	-	32.0 ⁶
36	6.1 ⁶	-	-	-	-	6.1 ⁶
42	50.7 ⁶	-	-	-	-	50.7 ⁶
48	20.1 ⁶	-	-	-	-	20.1 ⁶
average	37.6 ⁴⁴	33.7 ¹³	11.8 ¹⁴	12.0 ⁵	5.6 ¹¹	33.2 ⁸⁷

Table 11. Results for vapor pressure estimation (RMD) of triglycerides with Nannoolal / Rarey / Ramjugernath / estimated T_b model. The number in superscript is the number of data points used. The two substances –CH₂– 18 and 24 were excluded from average.

pressure region	I	II	III	IV	V	
–CH ₂ –	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	30.1 ²	31.7 ⁵	34.9 ⁴	43.3 ⁶	36.3 ¹⁷
3	72.8 ²	71.7 ³	-	-	37.9 ¹	66.5 ⁶
6	75.6 ⁶	67.2 ⁴	48.9 ⁶	-	33.3 ²	60.1 ¹⁸
12	83.9 ⁶	77.3 ⁴	65.0 ³	68.6 ¹	59.4 ²	74.7 ¹⁶
15	79.2 ⁶	-	-	-	-	79.2 ⁶
(18)	(82.3 ⁸)	(83.2 ⁵)	(83.9 ³)	(90.3 ²)	(85.5 ²)	(83.9 ²⁰)
(24)	(87.6 ⁶)	-	-	-	-	(87.6 ⁶)
30	93.0 ⁶	-	-	-	-	93.0 ⁶
36	95.1 ⁶	-	-	-	-	95.1 ⁶
42	97.5 ⁶	-	-	-	-	97.5 ⁶
48	99.2 ⁶	-	-	-	-	99.2 ⁶
average	87.1 ⁴⁴	61.6 ¹³	48.5 ¹⁴	51.7 ⁵	43.5 ¹¹	78.0 ⁸⁷

Table 12. Results for vapor pressure estimation (RMD) of triglycerides with Ceriani (2013) model. The number in superscript is the number of data points used. Due to a missing group, application to –CH₂– 3 (Triisovalerin) was not possible.

pressure region	I	II	III	IV	V	
–CH ₂ –	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	23.2 ²	59.0 ⁵	96.8 ⁴	167.4 ⁶	101.9 ¹⁷
3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
6	72.9 ⁶	39.1 ⁴	8.1 ⁶	-	45.0 ²	40.7 ¹⁸
12	49.5 ⁶	38.3 ⁴	13.1 ³	24.2 ¹	11.7 ²	33.6 ¹⁶
15	28.1 ⁶	-	-	-	-	28.1 ⁶
18	8.8 ⁸	44.6 ⁵	56.5 ³	74.9 ²	67.8 ²	37.4 ²⁰
24	13.2 ⁶	-	-	-	-	13.2 ⁶

30	1.9 ⁶	-	-	-	-	1.9 ⁶
36	8.1 ⁶	-	-	-	-	8.1 ⁶
42	1.7 ⁶	-	-	-	-	1.7 ⁶
48	28.1 ⁶	-	-	-	-	28.1 ⁶
average	23.6 ⁵⁶	36.3 ¹⁵	34.2 ¹⁷	65.3 ⁷	72.9 ¹²	29.5 ¹⁰⁷

Chapter 3.1.1: Detailed results for vapor pressure estimation of triglycerides using the set of revised T_b

Tables 13-15 show detailed results for vapor pressure estimations for each model.

Table 13. Results for vapor pressure estimation of triglycerides with Moller / Rarey / Ramjugernath model using the set of revised T_b . The number in superscript is the number of data points used.

pressure region	I	II	III	IV	V	
–CH ₂ –	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	0.4 ²	0.3 ⁵	0.8 ⁴	11.5 ⁶	4.4 ¹⁷
3	43.9 ²	20.8 ³	-	-	55.7 ¹	34.3 ⁶
6	56.0 ⁶	16.0 ⁴	34.6 ⁶	-	41.9 ²	38.4 ¹⁸
12	57.4 ⁶	11.3 ⁴	20.6 ³	2.3 ¹	13.4 ²	30.0 ¹⁶
15	56.8 ⁶	-	-	-	-	56.8 ⁶
18	54.1 ⁸	24.0 ⁵	39.4 ³	65.0 ²	54.0 ²	45.4 ²⁰
24	66.5 ⁶	-	-	-	-	66.5 ⁶
30	79.4 ⁶	-	-	-	-	79.4 ⁶
36	93.7 ⁶	-	-	-	-	93.7 ⁶
42	109.8 ⁶	-	-	-	-	109.8 ⁶
48	135.9 ⁶	-	-	-	-	135.9 ⁶
average	75.3 ⁵⁸	14.5 ¹⁸	23.7 ¹⁷	22.7 ⁷	35.3 ¹³	63.2 ¹¹³

Table 14. Results for vapor pressure estimation of triglycerides with Nannoolal / Rarey / Ramjugernath model using the set of revised T_b . The number in superscript is the number of data points used.

pressure region	I	II	III	IV	V	
–CH ₂ –	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	10.7 ²	6.4 ⁵	1.7 ⁴	13.2 ⁶	8.2 ¹⁷
3	19.8 ²	13.9 ³	-	-	59.4 ¹	23.5 ⁶
6	28.0 ⁶	11.5 ⁴	26.0 ⁶	-	44.7 ²	25.5 ¹⁸

12	32.7 ⁶	15.1 ⁴	12.6 ³	2.6 ¹	14.3 ²	20.3 ¹⁶
15	35.0 ⁶	-	-	-	-	35.0 ⁶
18	33.9 ⁸	34.3 ⁵	45.7 ³	68.1 ²	56.1 ²	41.4 ²⁰
24	35.4 ⁶	-	-	-	-	35.4 ⁶
30	34.5 ⁶	-	-	-	-	34.5 ⁶
36	34.8 ⁶	-	-	-	-	34.8 ⁶
42	33.2 ⁶	-	-	-	-	33.2 ⁶
48	33.4 ⁶	-	-	-	-	33.4 ⁶
average	32.1 ⁵⁸	17.1 ¹⁸	22.7 ¹⁷	24.1 ⁷	37.5 ¹³	29.6 ¹¹³

Table 15. Results for vapor pressure estimation of triglycerides with Ceriani (2013) model using the set of revised T_b . The number in superscript is the number of data points used.

pressure region	I	II	III	IV	V	
–CH₂–	< 1 kPa	1 kPa to < 10 kPa	10 kPa to < 40 kPa	40 kPa to 100 kPa	> 100 kPa	overall
0	-	23.2 ²	59.0 ⁵	96.8 ⁴	167.4 ⁶	101.9 ¹⁷
3	-	-	-	-	-	-
6	72.9 ⁶	39.1 ⁴	8.1 ⁶	-	45.0 ²	40.7 ¹⁸
12	49.5 ⁶	38.3 ⁴	13.1 ³	24.2 ¹	11.7 ²	33.6 ¹⁶
15	28.1 ⁶	-	-	-	-	28.1 ⁶
18	8.8 ⁸	44.6 ⁵	56.5 ³	74.9 ²	67.8 ²	37.4 ²⁰
24	13.2 ⁶	-	-	-	-	13.2 ⁶
30	1.9 ⁶	-	-	-	-	1.9 ⁶
36	8.1 ⁶	-	-	-	-	8.1 ⁶
42	1.7 ⁶	-	-	-	-	1.7 ⁶
48	28.1 ⁶	-	-	-	-	28.1 ⁶
average	23.6 ⁵⁸	36.3 ¹⁸	34.2 ¹⁷	65.3 ⁷	72.9 ¹³	29.5 ¹¹³