



# Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of *n*-Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane

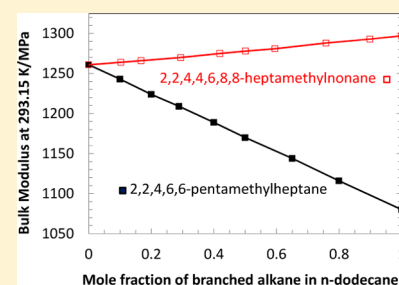
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## S Supporting Information

**ABSTRACT:** In this work, the physical properties of binary mixtures of *n*-dodecane with 2,2,4,6,6-pentamethylheptane or 2,2,4,4,6,8,8-heptamethylnonane were measured and compared to properties of four hydrotreated renewable jet (HRJ) and hydrotreated renewable diesel (HRD) fuels. Density and viscosity were measured at temperatures ranging from (293.15 to 393.15) K, and the speed of sound was measured at temperatures ranging from (293.15 to 333.15) K. For the mixtures, the speed of sound at 293.15 K decreased (1297.6 to 1285.7) m·s<sup>-1</sup> as the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane increased and decreased (1297.6 to 1203.6) m·s<sup>-1</sup> as the mole fraction of 2,2,4,6,6-pentamethylheptane increased. The bulk modulus was calculated from density and speed of sound data. Flash points for the mixtures ranged from (318 to 367) K, and surface tension values ranged from (21.8 to 25.3) mN·m<sup>-1</sup>. When comparing to alternative fuels, two-component mixtures could be found to match the density and viscosity of HRJs and HRDs. The mixtures matched the speed of sound, bulk modulus, surface tension, and flash point of some of these hydrotreated fuels. These data suggest that binary mixtures of *n*-dodecane with branched alkanes may be suitable surrogates for renewable fuels.



## 1. INTRODUCTION

Alternative fuels for use in diesel and jet engines can be derived from corn, sugar, algae, camelina, and waste products such as tallow. The oils derived from these sources can be reacted with hydrogen over a catalyst to remove the oxygen and to saturate the double bonds.<sup>1</sup> This process, called hydrotreating, produces a mixture containing predominantly branched and linear alkanes.<sup>2</sup> In a 2012 fleet demonstration, the U.S. Navy successfully powered ships using a 50:50 mixture of hydrotreated diesel (HRD-76) and petroleum F-76 diesel and flew aircraft with a 50:50 mixture of hydrotreated jet fuel (HRJ-5) and petroleum JP-5 aviation fuel.<sup>3</sup> The modeling of the combustion of these fuels requires many input parameters for the various fuel components. Researchers have sought to simplify the modeling and to understand the combustion of various fuels by developing surrogate mixtures, which have a small number of known components, that match the physical and combustion properties of the fuel of interest.<sup>4–23</sup>

Some of the physical properties of hydrotreated renewable fuels (HRFs) have been matched using surrogate mixtures containing one or more linear alkanes such as *n*-pentadecane, *n*-hexadecane, *n*-heptadecane, and *n*-octadecane mixed with a branched alkane such as 2-methyloctane, 2-methylnonane, 2,2,4-trimethylpentane (isooctane), 2,2,4,4,6,8,8-heptanemethylnonane (isocetane), 2,2,4,6,6-pentamethylheptane, or with a blend of isododecane isomers.<sup>5–8,23</sup> Several of these surrogate mixtures have been shown to have similar combustion behavior to the HRFs when tested in military diesel engines.<sup>5,6,8</sup> In this

work, the physical properties of new surrogate mixtures containing *n*-dodecane with 2,2,4,6,6-pentamethylheptane or 2,2,4,4,6,8,8-heptanemethylnonane were measured and compared with those previously reported for hydrotreated renewable diesel fuel from algae (algal HRD-76), hydrotreated renewable jet fuels from camelina (camelina HRJ-5), and tallow (tallow HRJ-5), and to a direct sugar to hydrocarbon diesel fuel (DSH-76) to determine if they could potentially be suitable surrogate mixtures for these fuels.<sup>7,23,24</sup>

The physical properties used in the development of surrogate mixtures include those that impact the physical transport of the fuel into the combustion chamber, as well the physical and chemical processes in the combustion chamber itself. Some commonly measured properties are density, speed of sound, bulk modulus, viscosity, and distillation curve.<sup>4,5,9,11,14,16,23</sup> The bulk modulus, which is calculated from density and speed of sound measurements, directly affects fuel injection time.<sup>5,25</sup> The viscosity, surface tension, and density have been used as input parameters in the simulation of the vaporization of multicomponent fuel droplets.<sup>26</sup> Previous studies have measured the density, viscosity, speed of sound, surface tension, and flash point and have determined the bulk modulus of binary mixtures of *n*-hexadecane with 2,2,4,6,6-pentamethylheptane and 2,2,4,4,6,8,8-heptanemethylnonane.<sup>7,23</sup> These

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studies have included flash point because it is part of the specifications for military diesel fuel.<sup>27</sup> In this work, these same properties are measured for binary mixtures of *n*-dodecane with the same branched alkanes, 2,2,4,6,6-pentamethylheptane and 2,2,4,4,6,8,8-heptamethylnonane.

## 2. MATERIALS

The *n*-dodecane, 2,2,4,4,6,8,8-heptamethylnonane, and 2,2,4,6,6-pentamethylheptane were used as received from supplier (Table 1). Mixtures of *n*-hexadecane and a branched

alkane were prepared at 293.15 K by weighing each component on a Mettler Toledo AG204 analytical balance. The scale was calibrated using the internal calibration weight on the instrument. The manufacturer reports that the balance has a standard deviation of 0.0001 g, while actual measurements suggest a higher value of around 0.0005 g. Through a propagation of error using a standard deviation of 0.0005 g for mass and the molar masses of 2,2,4,4,6,8,8-heptamethylnonane and 2,2,4,6,6-pentamethylheptane with their associated errors from Harris,<sup>28</sup> a standard deviation for mole fraction was calculated and multiplied by 2 (for a 95 % confidence interval and assuming a normal distribution) to yield a combined expanded uncertainty for molar mass of 0.0001.

## 3. METHODS

A DSA 5000 density and sound analyzer (Anton Paar) was used to measure the speed of sound and the density of the mixtures at five temperatures between (293.15 and 333.15) K, while an SVM 3000 Stabinger viscometer (Anton Paar) was used to measure the viscosity and also density of the mixtures at

**Table 1. Sample Information**

chemical name	source	mole fraction purity	analysis method
<i>n</i> -dodecane	Aldrich	0.995	GC <sup>a</sup>
2,2,4,6,6-pentamethylheptane	TCI	> 0.98	GC <sup>a</sup>
2,2,4,4,6,8,8-heptamethylnonane	Aldrich	≥ 0.994	GC <sup>a</sup>

<sup>a</sup>Gas–liquid chromatography.

**Table 2. Experimental Values of Density  $\rho$  (kg·m<sup>-3</sup>), Dynamic Viscosity  $\eta$  (mPa·s), and Kinematic Viscosity  $\nu$  (mm<sup>2</sup>·s<sup>-1</sup>) of Mixtures of 2,2,4,4,6,8,8-Heptamethylnonane (1) + *n*-Dodecane from  $T = (293 \text{ to } 373)$  K and 0.1 MPa<sup>a</sup>**

$X_1$	$\rho$ kg·m <sup>-3</sup>	$\eta$ mPa·s	$\nu$ mm <sup>2</sup> ·s <sup>-1</sup>	$\rho$ kg·m <sup>-3</sup>	$\eta$ mPa·s	$\nu$ mm <sup>2</sup> ·s <sup>-1</sup>	$\rho$ kg·m <sup>-3</sup>	$\eta$ mPa·s	$\nu$ mm <sup>2</sup> ·s <sup>-1</sup>
	$T = 293.15 \text{ K}$			$T = 303.15 \text{ K}$			$T = 313.15 \text{ K}$		
0.0000	748.89(3)	1.49	1.99	741.63(5)	1.25	1.68	734.34(9)	1.06	1.44
0.1030	753.26(3)	1.59	2.10	746.09(2)	1.32	1.77	738.89(5)	1.12	1.51
0.1677	756.13(7)	1.67	2.21	749.06(5)	1.39	1.86	741.92(1)	1.17	1.58
0.2944	761.09(0)	1.84	2.42	754.06(8)	1.53	2.02	747.01(1)	1.28	1.72
0.4191	765.49(7)	2.03	2.65	758.54(0)	1.67	2.21	751.55(6)	1.40	1.87
0.5011	768.60(4)	2.19	2.86	761.70(2)	1.80	2.36	754.77(0)	1.50	1.99
0.5955	771.81(9)	2.40	3.11	764.96(4)	1.95	2.55	758.08(5)	1.63	2.14
0.7585	777.12(8)	2.83	3.64	770.34(6)	2.28	2.96	763.53(8)	1.88	2.46
0.8985	781.52(7)	3.29	4.21	774.79(0)	2.62	3.38	768.02(8)	2.14	2.79
1.0000	784.45(7)	3.70	4.72	777.76(1)	2.92	3.76	771.04(4)	2.37	3.07
	$T = 323.15 \text{ K}$			$T = 333.15 \text{ K}$			$T = 343.15 \text{ K}$		
0.0000	727.03(8)	0.916	1.26	719.69(1)	0.799	1.11	712.2	0.704	0.98(9)
0.1030	731.66(9)	0.966	1.32	724.40(7)	0.840	1.16	717.1	0.738	1.03
0.1677	734.74(9)	1.01	1.38	727.54(0)	0.877	1.21	720.2	0.769	1.07
0.2944	739.92(6)	1.10	1.48	732.80(5)	0.950	1.30	725.6	0.830	1.14
0.4191	744.54(6)	1.19	1.60	737.50(3)	1.03	1.39	730.4	0.895	1.23
0.5011	747.81(2)	1.27	1.70	740.82(1)	1.09	1.47	733.7	0.949	1.29
0.5955	751.18(0)	1.37	1.82	744.24(4)	1.17	1.57	737.2	1.01	1.37
0.7585	756.70(8)	1.57	2.07	749.85(8)	1.33	1.77	743.0	1.14	1.54
0.8985	761.26(6)	1.77	2.32	754.48(4)	1.49	1.97	747.6	1.27	1.70
1.0000	764.31(6)	1.95	2.55	757.57(1)	1.63	2.15	750.7	1.39	1.85
	$T = 353.15 \text{ K}$			$T = 363.15 \text{ K}$			$T = 373.15 \text{ K}$		
0.0000	704.7	0.625	0.88(7)	697.1	0.560	0.80(3)	689.6	0.506	0.73(4)
0.1030	709.6	0.654	0.92(2)	702.0	0.585	0.83(3)	694.5	0.528	0.76(0)
0.1677	712.7	0.681	0.95(5)	705.3	0.608	0.86(2)	697.8	0.548	0.78(5)
0.2944	718.2	0.732	1.02	710.8	0.652	0.91(7)	703.5	0.586	0.83(3)
0.4191	723.1	0.787	1.09	715.8	0.698	0.98(7)	708.5	0.626	0.88(3)
0.5011	726.5	0.832	1.14	719.2	0.737	1.02	712.0	0.659	0.92(6)
0.5955	730.1	0.885	1.21	722.9	0.782	1.08	715.8	0.697	0.97(4)
0.7585	736.0	0.994	1.35	728.9	0.873	1.20	721.8	0.775	1.07
0.8985	740.7	1.10	1.49	733.6	0.963	1.31	726.6	0.850	1.17
1.0000	743.8	1.19	1.60	736.8	1.04	1.41	729.9	0.914	1.25

<sup>a</sup> $X_1$  is the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane in the (2,2,4,4,6,8,8-heptamethylnonane + *n*-dodecane) mixture. The standard uncertainty  $u$  is  $u(T) = 0.01 \text{ K}$ , and combined expanded uncertainties  $U_c$  are  $U_c(\rho) = 0.5 \text{ kg·m}^{-3}$ ,  $U_c(\eta) = 0.008 \text{ mPa·s}$ ,  $U_c(\nu) = 0.01 \text{ mm}^2\text{·s}^{-1}$  (level of confidence = 0.95,  $k \approx 2$ ).

Table 3. Comparison of the Measured Property Values with Literature Values

compound	property	T/K	this study		literature
2,2,4,4,6,8,8-heptamethylnonane	$\rho/\text{kg}\cdot\text{m}^{-3}$	293.15	$784.46 \pm 0.5$	$784.5 \pm 0.3^7$	
		313.15	$771.04 \pm 0.5$	$771.0 \pm 0.3^7$	
		333.15	$757.57 \pm 0.5$	$757.4 \pm 0.3^7$	
		353.15	$743.8 \pm 0.5$	$743.8 \pm 0.3^7$	
		373.15	$729.9 \pm 0.5$	$730.3 \pm 0.3^7$	
	$\mu/\text{mPa}\cdot\text{s}$	293.15	$3.70 \pm 0.008$	$3.70 \pm 0.34^7$	
		313.15	$2.37 \pm 0.008$	$2.37 \pm 0.04^7$	
		333.15	$1.63 \pm 0.008$	$1.63 \pm 0.04^7$	
		353.15	$1.19 \pm 0.008$	$1.19(7) \pm 0.04^7$	
		373.15	$0.914 \pm 0.008$	$0.918 \pm 0.04^7$	
	$c/\text{m}\cdot\text{s}^{-1}$	293.15	$1285.7 \pm 0.3$	$1285.9 \pm 0.3^7$	
		303.15	$1248.5 \pm 0.3$	$1248.6 \pm 0.3^7$	
		313.15	$1211.8 \pm 0.3$	$1211.9 \pm 0.3^7$	
		323.15	$1176.0 \pm 0.3$	$1176.0 \pm 0.3^7$	
	surface tension/ $\text{mN}\cdot\text{m}^{-1}$	294.7	$24.0 \pm 0.2$	$24.1 \pm 0.2^7$	
2,2,4,6,6-pentamethylheptane	$c/\text{m}\cdot\text{s}^{-1}$	293.15	$1203.6 \pm 0.3$	$1204.0 \pm 0.3^{23}$	
		303.15	$1164.8 \pm 0.3$	$1164.9 \pm 0.3^{23}$	
		313.15	$1126.7 \pm 0.3$	$1126.7 \pm 0.3^{23}$	
		323.15	$1089.3 \pm 0.3$	$1089.3 \pm 0.3^{23}$	
<i>n</i> -dodecane	$\mu/\text{mPa}\cdot\text{s}$	293.15	$1.49 \pm 0.008$	$1.48 \pm 0.1 \%,^{34} 1.4885,^{36} 1.50 \pm 1 \%^{35}$	
		303.15	$1.25 \pm 0.008$	$1.2315 \pm 2 \%,^{37} 1.2328 \pm 0.05 \%,^{38} 1.2462^{36}$	
		313.15	$1.06 \pm 0.008$	$1.0610,^{36} 1.062 \pm 0.1 \%,^{34} 1.07 \pm 1 \%^{35}$	
		323.15	$0.916 \pm 0.008$	$0.891,^{39} 0.9100 \pm 2 \%,^{37} 0.91600^{36}$	
		333.15	$0.799 \pm 0.008$	$0.080022,^{36} 0.8041 \pm 0.05 \%,^{40} 0.8048 \pm 0.12 \%,^{40} 0.81 \pm 1 \%^{35}$	
		353.15	$0.625 \pm 0.008$	$0.62490,^{36} 0.634 \pm 1 \%^{35}$	
	$c/\text{m}\cdot\text{s}^{-1}$	303.15	$1259.3 \pm 0.3$	$1260.9,^{42} 1261.2^{36}$	
		333.15	$1147.5 \pm 0.3$	$1147.4,^{42} 1146.6^{36}$	
	flash point/K		$354 \pm 2$	$352 \text{ K}^{49} \text{ and } 358 \pm 2^{50}$	

nine temperatures between (293.15 and 373.15) K. For the DSA 5000, the instrument was cleaned and calibrated each day using distilled water as specified by the manufacturer. Two or more samples of each individual liquid or liquid mixture were measured, and these replicates were used to determine the standard deviation. The accuracy of the SVM 3000 was tested using a NIST certified viscosity/density reference standard (Standard S3, Cannon Instrument Company) for higher density and viscosity values and *n*-decane for the lower density and viscosity values. If the density deviated by more than 0.1 % from the reference value or if the viscosity deviated by more than 1 % from the reference value, then the instrument was cleaned and retested. Two or more samples of each individual liquid or liquid mixture were measured, and these replicate measurements were used to determine the standard deviation of the measurement.

The surface tension of the liquids was measured using an axisymmetric drop shape analyzer (Kruss DS100). In this instrument, a liquid droplet of the fuel or fuel mixture was formed in air using a syringe and needle of known diameter. An image of the droplet was taken and magnified. This image was then fit using the Young–LaPlace equation within input parameters of the needle diameter and the densities of the air and the organic phase to determine the surface tension.<sup>29,30</sup> Over 15 surface tension measurements were taken for three droplets or more of each liquid as has been done in previous studies, and these values were used to calculate the standard deviation of each measurement.<sup>5,7,23</sup>

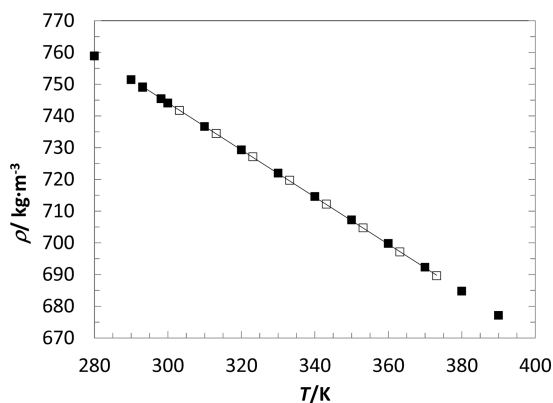
The flash points of the mixtures were measured using a Setaflash Series 8 closed cup flash point tester model 82000-0 (Stanhope-Seta) using a temperature ramping setting. The

manufacturer's literature specifies that this flash point tester conforms to ASTM D3828 (gas ignition option), ASTM D1655 (gas ignition option), ASTM D3278, ASTM D7236, and ASTM E502. Two measurements were taken for each mixture from which the average and standard deviation were determined.

To determine the combined expanded uncertainty of density, viscosity, speed of sound, surface tension, and flash point, the standard deviation of the measurements taken at each temperature as described above were multiplied by 2. When a normal distribution is assumed, multiplying by a coverage factor of 2 produces in a 95 % confidence interval. Since the purity of the 2,2,4,6,6-pentamethylheptane is only 0.98 or greater, the combined expanded uncertainty is larger than suggested by the precision of the measurements.<sup>53</sup> In the case of density, the combined expanded uncertainty is  $1 \text{ kg}\cdot\text{m}^{-3}$ . For the 2,2,4,4,6,8,8-heptamethylnonane and *n*-dodecane, whose purity is greater than 0.994, the combined expanded uncertainty is  $0.5 \text{ kg}\cdot\text{m}^{-3}$ .

## 4. RESULTS

**4.1. Density.** The density values of 2,2,4,4,6,8,8-heptamethylnonane, *n*-dodecane, and their mixtures are given in Table 2 as a function of the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane ( $X_1$ ). The densities of 2,2,4,4,6,8,8-heptamethylnonane agree with measured values<sup>7</sup> as shown in Table 3. The densities of *n*-dodecane agree with the values recommended by Marsh,<sup>31</sup> which are based on a compilation of over 13 references, as shown in Figure 1. The density values of 2,2,4,6,6-pentamethylheptane, *n*-dodecane, and their mixtures are given in Table 4 as a function of the mole fraction of



**Figure 1.** Density of *n*-dodecane: □, this study; ■, ref 31. Error bars, which are the combined expanded uncertainties with 0.95 level of confidence ( $k \approx 2$ ), are smaller than symbols.

2,2,4,6,6-pentamethylheptane ( $X_1$ ). The density values for 2,2,4,6,6-pentamethylheptane were taken from Luning Prak et al.<sup>23</sup>

For the mixtures, the density increased as mole fraction of 2,2,4,4,6,8,8-heptamethylnonane increased, but the increase was

not linear as shown in Figure 2. A second-order polynomial was used to fit the density and mole fraction data:

$$\rho/\text{kg}\cdot\text{m}^{-3} = AX_1^2 + BX_1 + C \quad (1)$$

In this equation  $X_1$  is the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane, and  $A$ ,  $B$ , and  $C$  are fitting parameters, which are given in Table 5. The fit was conducted using Microsoft Excel 2010. The standard error of a fit,  $\sigma$ , of a parameter,  $P$ , can be represented by represented by<sup>32</sup>

$$\sigma = \sqrt{\frac{\sum (P_{\text{measured}} - P_{\text{fit}})^2}{N - n}} \quad (2)$$

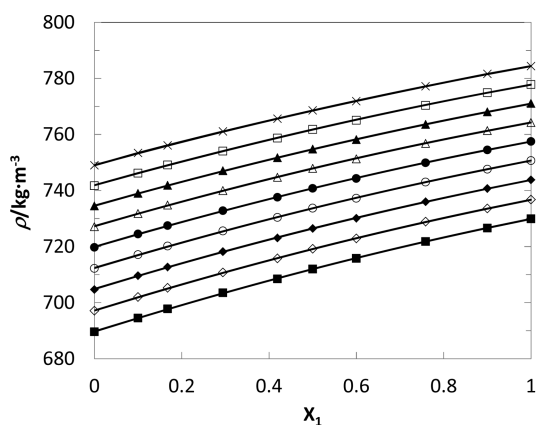
where  $P_{\text{measured}}$  is the measured parameter, such as density,  $P_{\text{fit}}$  is the fitted value, such as fitted density,  $N$  is the number of data points, and  $n$  is the number of fitting parameters. The standard errors for the density fits are given in Table 5. The fits are good with  $R^2 > 0.9999$  as shown in Figure 2.

For the mixtures containing 2,2,4,6,6-pentamethylheptane and *n*-dodecane, the density decreased as mole fraction of 2,2,4,6,6-pentamethylheptane increased, and the decrease appears to be linear as shown in Figure 3. Both the nonlinear model, eq 1, and a linear model:

**Table 4.** Experimental Values of Density  $\rho$  ( $\text{kg}\cdot\text{m}^{-3}$ ), Dynamic Viscosity  $\eta$  (mPa·s), and Kinematic Viscosity  $\nu$  ( $\text{mm}^2\cdot\text{s}^{-1}$ ) of Mixtures of 2,2,4,6,6-Pentamethylheptane (1) + *n*-Dodecane from  $T = (293 \text{ to } 373) \text{ K}$  and  $0.1 \text{ MPa}^a$

$X_1$	$\rho$ kg·m <sup>-3</sup>	$\eta$ mPa·s	$\nu$ mm <sup>2</sup> ·s <sup>-1</sup>	$\rho$ kg·m <sup>-3</sup>	$\eta$ mPa·s	$\nu$ mm <sup>2</sup> ·s <sup>-1</sup>	$\rho$ kg·m <sup>-3</sup>	$\eta$ mPa·s	$\nu$ mm <sup>2</sup> ·s <sup>-1</sup>
	$T = 293.15 \text{ K}$			$T = 303.15 \text{ K}$			$T = 313.15 \text{ K}$		
0.0000	748.89(3)	1.49	1.99	741.63(5)	1.25	1.68	734.34(9)	1.06	1.44
0.1000	748.46(7)	1.45	1.94	741.23(4)	1.22	1.64	733.97(0)	1.03	1.41
0.2000	748.12(3)	1.42	1.90	740.89(8)	1.20	1.62	733.64(0)	1.02	1.38
0.2885	747.85(7)	1.40	1.87	740.65(4)	1.18	1.60	733.41(5)	1.00	1.37
0.3998	747.38(7)	1.37	1.83	740.15(0)	1.16	1.57	732.95(3)	0.988	1.35
0.4999	747.03(4)	1.35	1.81	739.83(5)	1.15	1.55	732.59(8)	0.977	1.33
0.6501	746.51(9)	1.33	1.78	739.31(3)	1.13	1.53	732.06(6)	0.962	1.31
0.7998	745.94(7)	1.31	1.76	738.71(5)	1.12	1.51	731.44(5)	0.952	1.30
1.0000 <sup>b</sup>	745.5	1.29	1.74	738.2	1.10	1.49	730.9	0.941	1.29
	$T = 323.15 \text{ K}$			$T = 333.15 \text{ K}$			$T = 343.15 \text{ K}$		
0.0000	727.03(8)	0.916	1.26	719.69(1)	0.799	1.11	712.2	0.704	0.989
0.1000	726.67(4)	0.898	1.24	719.34(2)	0.784	1.09	711.9	0.691	0.970
0.2000	726.35(2)	0.885	1.22	719.02(4)	0.774	1.08	711.7	0.683	0.960
0.2885	726.13(9)	0.876	1.21	718.82(0)	0.766	1.07	711.5	0.677	0.952
0.3998	725.68(0)	0.863	1.19	718.36(3)	0.757	1.05	710.9	0.668	0.940
0.4999	725.32(4)	0.856	1.18	718.00(4)	0.750	1.05	710.6	0.664	0.935
0.6501	724.78(1)	0.844	1.16	717.44(9)	0.741	1.03	710.0	0.656	0.924
0.7998	724.13(6)	0.836	1.15	716.78(3)	0.734	1.02	709.4	0.651	0.917
1.0000 <sup>b</sup>	723.5	0.82(7)	1.14	716.1	0.72(6)	1.01	708.6	0.64(3)	0.90(8)
	$T = 353.15 \text{ K}$			$T = 363.15 \text{ K}$			$T = 373.15 \text{ K}$		
0.0000	704.7	0.625	0.887	697.1	0.560	0.803	689.6	0.506	0.734
0.1000	704.4	0.614	0.872	696.8	0.551	0.790	689.0	0.498	0.723
0.2000	704.1	0.607	0.863	696.5	0.545	0.782	688.8	0.493	0.716
0.2885	703.8	0.603	0.856	696.3	0.526	0.777	688.6	0.490	0.711
0.3998	703.5	0.595	0.846	695.8	0.534	0.767	688.1	0.483	0.703
0.4999	703.0	0.591	0.841	695.4	0.531	0.764	687.7	0.481	0.700
0.6501	702.5	0.584	0.832	694.8	0.525	0.755	687.1	0.476	0.692
0.7998	701.8	0.580	0.826	694.1	0.521	0.751	686.3	0.472	0.688
1.0000 <sup>b</sup>	700.9	0.57(3)	0.81(8)	693.2	0.51(5)	0.74(3)	685.5	0.46(7)	0.68(1)

<sup>a</sup> $X_1$  is the mole fraction of 2,2,4,6,6-pentamethylheptane (1) in (2,2,4,6,6-pentamethylheptane + *n*-dodecane). The standard uncertainty  $u$  is  $u(T) = 0.01 \text{ K}$ , and combined expanded uncertainties  $U_c$  are  $U_c(\rho) = 1 \text{ kg}\cdot\text{m}^{-3}$ ,  $U_c(\eta) = 0.005 \text{ mPa}\cdot\text{s}$ ,  $U_c(\nu) = 0.007 \text{ mm}^2\cdot\text{s}^{-1}$  (level of confidence = 0.95,  $k \approx 2$ ). <sup>b</sup>Data for pure 2,2,4,6,6-pentamethylheptane was taken from Luning Prak et al.<sup>23</sup>

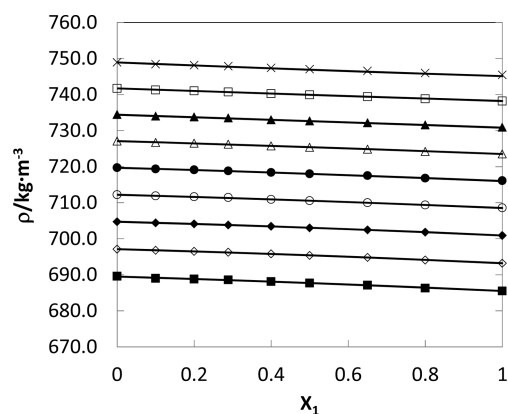


**Figure 2.** Density of 2,2,4,4,6,8,8-heptamethylnonane ( $X_1$ ) +  $n$ -dodecane mixtures at  $\times$ , 293.15 K;  $\square$ , 303.15 K;  $\blacktriangle$ , 313.15 K;  $\triangle$ , 323.15 K;  $\bullet$ , 333.15 K;  $\circ$ , 343.15 K;  $\blacklozenge$ , 353.15 K;  $\diamond$ , 363.15 K;  $\blacksquare$ , 373.15 K. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ), are smaller than the symbols. Lines shown are second-order fits using eq 1 with the coefficients in Table 4.

$$\rho/\text{kg}\cdot\text{m}^{-3} = DX_1 + E \quad (3)$$

were used to fit the density and mole fraction data. In this equation  $X_1$  is the mole fraction of 2,2,4,6,6-pentamethylheptane, and  $D$  and  $E$  are fitting parameters. The fitting parameters for both models are given in Table 6. The fit was conducted using Microsoft Excel 2010, and the standard error of each fit is given by eq 2. The fits using both models are good with  $R^2 > 0.99$ , and the fit for the polynomial model is shown in Figure 3. At the low temperatures of (293.15 to 333.15) K, the values of  $A$  in eq 1 have error bars that overlap with zero, and the standard errors for the linear fits are similar to those of the polynomial fits at (303.15 and 313.15) K. Above 333.15 K, the standard errors of the polynomial fits are lower than those of the linear fit, suggesting that the polynomial fit is better than the linear fit at these temperatures.

To determine if the solutions deviated from ideal solution behavior, the excess molar volumes were calculated. An ideal solution would have an excess molar volume equal to zero.



**Figure 3.** Density of 2,2,4,6,6-pentamethylheptane ( $X_1$ ) +  $n$ -dodecane mixtures at  $\times$ , 293.15 K;  $\square$ , 303.15 K;  $\blacktriangle$ , 313.15 K;  $\triangle$ , 323.15 K;  $\bullet$ , 333.15 K;  $\circ$ , 343.15 K;  $\blacklozenge$ , 353.15 K;  $\diamond$ , 363.15 K;  $\blacksquare$ , 373.15 K. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ), are smaller than the symbols. Lines shown are second-order fits using eq 1 with the coefficients in Table 5.

Fermeglia and Torriano<sup>32</sup> showed that excess molar volumes of two-component mixtures of 2,2,4,4,6,8,8-heptamethylnonane with  $n$ -hexadecane deviated the most from zero at mole fractions close to 0.5 at 298 K. In the current study, the excess molar volumes ( $V_m^E$ ) of 2,2,4,4,6,8,8-heptamethylnonane in  $n$ -dodecane were calculated at various temperatures for the 2,2,4,4,6,8,8-heptamethylnonane mole fraction of 0.5011 using the following equation:<sup>32</sup>

$$V_m^E = \frac{M_1X_1 + M_2X_2}{\rho_m} - \frac{M_1X_1}{\rho_1} - \frac{M_2X_2}{\rho_2} \quad (4)$$

where  $\rho_m$  is the density of the mixture,  $\rho_1$  and  $\rho_2$  are the densities,  $M_1$  and  $M_2$  are the molar masses, and  $X_1$  and  $X_2$  are the mole fractions of 2,2,4,4,6,8,8-heptamethylnonane as component 1 and  $n$ -dodecane as component 2. These calculated excess molar volumes are given in Table 5. The excess molar volumes of 2,2,4,6,6-pentamethylheptane in  $n$ -dodecane were also calculated at various temperatures for the 2,2,4,6,6-pentamethylheptane mole fraction of 0.4999 using eq 4, and these results are given in Table 6.

**Table 5.** Parameters for eq 1,  $\rho/\text{kg}\cdot\text{m}^{-3} = AX_1^2 + BX_1 + C$ , That Correlates Density to Mole Fraction of 2,2,4,4,6,8,8-Heptamethylnonane (1) in (2,2,4,4,6,8,8-Heptamethylnonane +  $n$ -Dodecane) Mixtures, Standard Errors, and the Excess Molar Volume ( $V_m^E$ ) at  $X_1 = 0.5011$ ,  $T = (293 \text{ to } 373) \text{ K}$ , and  $0.1 \text{ MPa}^a$

$T/\text{K}$	$A$	$B$	$C$	$R^2$	$\sigma \cdot 10^1$	$V_m^E$
						$\text{cm}^3\cdot\text{mol}^{-1}$
293.15	$-7.4 \pm 0.6$	$42.8 \pm 0.6$	$749.1 \pm 0.1$	0.9999	0.71	$0.073^b$
303.15	$-7.8 \pm 0.8$	$43.8 \pm 0.9$	$741.9 \pm 0.2$	0.9999	1.0	$0.057^b$
313.15	$-7.9 \pm 0.8$	$44.4 \pm 0.8$	$734.6 \pm 0.2$	0.9999	0.93	$0.042^b$
323.15	$-8.4 \pm 0.9$	$45.5 \pm 1.0$	$727.3 \pm 0.2$	0.9999	1.1	$0.029^b$
333.15	$-8.6 \pm 0.8$	$46.3 \pm 0.9$	$719.9 \pm 0.2$	0.9999	1.0	$0.019^b$
343.15	$-8.7 \pm 1.1$	$47.1 \pm 1.1$	$712.4 \pm 0.2$	0.9999	1.3	$0.01^b$
353.15	$-8.7 \pm 0.8$	$47.7 \pm 0.9$	$704.9 \pm 0.2$	0.9999	1.0	$0.01^b$
363.15	$-8.9 \pm 1.0$	$48.5 \pm 1.1$	$697.2 \pm 0.2$	0.9999	1.2	$0.02^b$
373.15	$-8.9 \pm 1.0$	$49.2 \pm 1.0$	$689.7 \pm 0.2$	0.9999	1.2	$0.03^b$

<sup>a</sup>The error for the coefficients  $A$ ,  $B$ , and  $C$  represents is a 95 % confidence interval. <sup>b</sup>The standard deviation in the excess volume as calculated by propagating the errors for the molar masses, masses, and densities. For temperatures at 333.15 K and below, the standard deviation was  $0.03 \text{ cm}^3\cdot\text{mol}^{-1}$  and the combined expanded uncertainty  $0.06 \text{ cm}^3\cdot\text{mol}^{-1}$ . Above 333.15 K, the standard deviation was  $0.04 \text{ cm}^3\cdot\text{mol}^{-1}$ , and the combined expanded uncertainty is  $0.08 \text{ cm}^3\cdot\text{mol}^{-1}$ . These combined expanded uncertainties were calculated using a coverage factor of 2 (95 % confidence interval).



Table 6. Parameters for Parameters for eq 1,  $\rho/\text{kg}\cdot\text{m}^{-3} = AX_1^2 + BX_1 + C$ , and eq 3,  $\rho/\text{kg}\cdot\text{m}^{-3} = DX_1 + E$ , That Correlates Density to Mole Fraction of 2,2,4,6,6-Pentamethylheptane (1) in (2,2,4,6,6-Pentamethylheptane + *n*-Dodecane) Mixtures, Standard Errors, and the Excess Molar Volume ( $V_m^E$ ) at  $X_1 = 0.4999$ ,  $T = (293 \text{ to } 373) \text{ K}$ , and  $0.1 \text{ MPa}$ <sup>a</sup>

T/K	A	B	C	R <sup>2</sup>	$\sigma \cdot 10^2$	D	E	R <sup>2</sup>	$\sigma \cdot 10^2$	$V_m^E$ cm <sup>3</sup> ·mol <sup>-1</sup>
293.15	0.5 ± 0.6	-4.0 ± 0.6	748.9 ± 0.1	0.997	6.5	-3.5 ± 0.2	748.8 ± 0.1	0.995	8.2	0.050 <sup>b</sup>
303.15	0.1 ± 0.4	-3.6 ± 0.4	741.7 ± 0.1	0.998	4.8	-3.5 ± 0.1	741.7 ± 0.1	0.999	4.5	0.034 <sup>b</sup>
313.15	-0.1 ± 0.5	-3.5 ± 0.6	734.4 ± 0.1	0.997	6.1	-3.6 ± 0.1	734.4 ± 0.1	0.998	5.7	0.023 <sup>b</sup>
323.15	-0.4 ± 0.5	-3.2 ± 0.5	727.1 ± 0.1	0.998	5.7	-3.6 ± 0.2	727.2 ± 0.1	0.997	6.8	-0.008 <sup>b</sup>
333.15	-0.6 ± 0.4	-3.1 ± 0.4	719.8 ± 0.1	0.998	4.8	-3.6 ± 0.2	719.8 ± 0.1	0.996	7.4	-0.031 <sup>b</sup>
343.15	-0.8 ± 0.6	-2.9 ± 0.6	712.2 ± 0.1	0.997	6.2	-3.7 ± 0.3	712.3 ± 0.1	0.993	10	-0.06 <sup>b</sup>
353.15	-1.0 ± 0.2	-2.8 ± 0.2	704.7 ± 0.1	0.999	2.3	-3.8 ± 0.3	704.8 ± 0.1	0.993	10	-0.07 <sup>b</sup>
363.15	-1.0 ± 0.3	-2.9 ± 0.3	697.1 ± 0.1	0.999	3.8	-3.9 ± 0.3	697.3 ± 0.2	0.993	11	-0.07 <sup>b</sup>
373.15	-0.8 ± 0.9	-3.2 ± 0.9	689.5 ± 0.2	0.994	10	-4.0 ± 0.4	689.6 ± 0.2	0.991	12	-0.06 <sup>b</sup>

<sup>a</sup>The error for the coefficients A, B, C, D, and E represents a 95 % confidence interval. <sup>b</sup>The standard deviation in the excess volume as calculated by propagating the errors for the molar masses, masses, and densities. For temperatures at 333.15 K and below, the standard deviation was 0.03 cm<sup>3</sup>·mol<sup>-1</sup> and the combined expanded uncertainty 0.06 cm<sup>3</sup>·mol<sup>-1</sup>. Above 333.15 K, the standard deviation was 0.04 cm<sup>3</sup>·mol<sup>-1</sup>, and the combined expanded uncertainty is 0.08 cm<sup>3</sup>·mol<sup>-1</sup>. These were calculated using a coverage factor of 2 (95 % confidence interval).

For *n*-hexadecane mixtures at mole fractions of branched alkanes close to 0.5 at 293 K, the excess molar volume changes from negative values to positive values as the total number of carbons in the branched alkane increases. Steiger et al.<sup>33</sup> reported that the excess molar volumes of two-component mixtures of *n*-hexadecane with branched heptanes, octanes, and decanes became less negative as the carbon number increased. At a mole fraction of 0.5, the excess molar volumes were (-0.198 to -0.545), (-0.133 to -0.233), and (-0.035 to -0.077) cm<sup>3</sup>·mol<sup>-1</sup> for the branched heptanes, octanes, and decanes, respectively.<sup>33</sup> A positive excess molar volume of 0.03 cm<sup>3</sup>·mol<sup>-1</sup> was reported for *n*-hexadecane with a branched dodecane, 2,2,4,6,6-pentamethylheptane, at a mole fraction of 0.5620 at 293 K.<sup>23</sup> An even longer chain branched alkane, 2,2,4,4,6,8,8-heptamethylnonane, has a more positive excess molar volume of 0.11 cm<sup>3</sup>·mol<sup>-1</sup> at a mole fraction of 0.5035 in *n*-hexadecane, which was calculated based on data in Luning Prak et al. at 293.15 K.<sup>7</sup>

Mixtures of branched alkanes with *n*-dodecane appear to be following the same trend of transitioning from negative to positive values with an increase in total number of carbons in the branched alkane. Steiger et al.<sup>33</sup> found excess molar volumes of *n*-dodecane with branched heptanes ranged from (-0.177 to -0.102) cm<sup>3</sup>·mol<sup>-1</sup> at a mole fraction of 0.5 and 293.15 K. In the current study, the mixture of 2,2,4,6,6-pentamethylheptane with *n*-dodecane has a positive excess molar volume at 293.15 K of 0.050 ± 0.06 cm<sup>3</sup>·mol<sup>-1</sup>. For mixtures of *n*-dodecane with 2,2,4,4,6,8,8-heptamethylnonane, the excess molar volume, 0.073 ± 0.06 cm<sup>3</sup>·mol<sup>-1</sup>, is slightly more positive than that of 2,2,4,6,6-heptamethylnonane at 293.15 K; however the confidence intervals overlap. At 373.15 K, the transition from negative to positive occurs at a longer chain length with values of (-0.06 ± 0.08 and 0.03 ± 0.08) cm<sup>3</sup>·mol<sup>-1</sup> for 2,2,4,6,6-pentamethylheptane and 2,2,4,4,6,8,8-heptamethylnonane mixtures, respectively.

The density values for the hydrotreated renewable fuels fall within the density values of some of the mixtures measured herein. At 293.15 K, the density values of (753.7 ± 0.2, 764.4 ± 0.2, 769.8 ± 0.2, and 776.1 ± 1.3) kg·m<sup>-3</sup> for tallow HRJ-5, camelina HRJ-5, DSH-76, and algal HRD-76, respectively, fall within the density values of the mixtures of 2,2,4,4,6,8,8-heptamethylnonane in *n*-dodecane measured herein, (749.0 to 784.4) kg·m<sup>-3</sup>.<sup>7,23,24</sup> The hydrotreated renewable fuels all have

density values greater than the values for mixtures of 2,2,4,6,6-pentamethylheptane and *n*-dodecane, (749.0 to 745.5) kg·m<sup>-3</sup>, at 293.15 K.

**4.2. Viscosity.** The dynamic and kinematic viscosity values of 2,2,4,4,6,8,8-heptamethylnonane, *n*-dodecane, and their mixtures are given in Table 2 as a function of the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane ( $X_1$ ). The viscosity values of *n*-dodecane agree with literature values within the error of the measurement as shown in Table 3. The viscosity values of 2,2,4,4,6,8,8-heptamethylnonane in Table 3 agree with previously measured values<sup>7</sup> using the same apparatus at the same temperatures but with samples from different manufacturer lots. The viscosity values of 2,2,4,6,6-pentamethylheptane, *n*-dodecane, and their mixtures are given in Table 4 as a function of the mole fraction of 2,2,4,6,6-pentamethylheptane ( $X_1$ ). The viscosity values for 2,2,4,6,6-pentamethylheptane were taken from Luning Prak et al.<sup>23</sup>

The McAllister three-body model<sup>41</sup> was used to fit the kinematic viscosity data:

$$\begin{aligned} \ln \nu_m = & X_1^3 \ln \nu_1 + 3X_1^2 X_2 \ln \nu_{1,2} + 3X_1 X_2^2 \ln \nu_{2,1} \\ & + X_2^3 \ln \nu_2 - \ln \left( X_1 + X_2 \frac{M_2}{M_1} \right) \\ & + 3X_1^2 X_2 \ln \left( \frac{1}{3} \left( 2 + \frac{M_2}{M_1} \right) \right) + 3X_1 X_2^2 \ln \left( \frac{1}{3} \left( 1 + 2 \frac{M_2}{M_1} \right) \right) \\ & + X_2^3 \ln \left( \frac{M_2}{M_1} \right) \end{aligned} \quad (5)$$

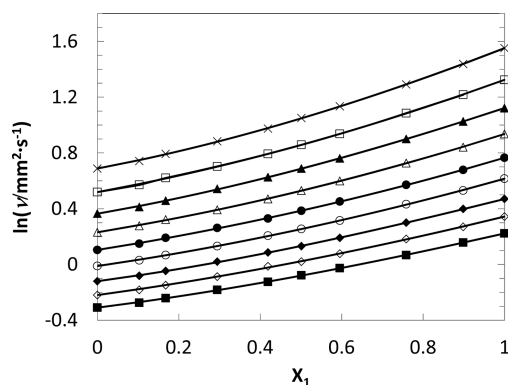
Here  $\nu_m$  is the kinematic viscosity of the binary mixture,  $X_1$  and  $X_2$  are the mole fractions,  $\nu_1$  and  $\nu_2$  are the kinematic viscosities of the pure components, and  $M_1$  and  $M_2$  are the molar masses of the branched alkane as component 1 and *n*-dodecane as component 2. The interaction parameters  $\nu_{2,1}$  and  $\nu_{1,2}$  were determined using the GRG nonlinear engine of the SOLVER function in Microsoft Excel 2010 to minimize the sum of the square of the difference between the value calculated by the model in eq 5,  $\nu_{m,\text{calc}}$  and the measured kinematic viscosity of the binary mixture,  $\nu_{\text{measured}}$ :

$$\min \sum (\nu_{m,\text{calc}} - \nu_{\text{measured}})^2 \quad (6)$$

The standard error for the fit ( $\sigma$ ) was determined by eq 2, where  $P_{\text{measured}}$  is the measured viscosity and  $P_{\text{fit}}$  is the fitted viscosity. The fitted values of  $\nu_{2,1}$  and  $\nu_{1,2}$  and the standard errors of the fits are given in Table 7 for each temperature. The model fits the data well as shown in Figures 4 and 5.

**Table 7. Values of the Coefficients for the McAllister Equation (eq 5) and Associated Standard Errors for Binary Mixtures of *n*-Dodecane with 2,2,4,4,6,8,8-Heptamethylnonane or 2,2,4,6,6-Pentamethylheptane from  $T = (293 \text{ to } 373) \text{ K}$**

$T/\text{K}$	2,2,4,4,6,8,8-heptamethylnonane mixtures			2,2,4,6,6-pentamethylheptane mixtures		
	$\nu_{12}$ $\text{mm}^2\cdot\text{s}^{-1}$	$\nu_{21}$ $\text{mm}^2\cdot\text{s}^{-1}$	$\sigma\cdot 10^3$ $\text{mm}^2\cdot\text{s}^{-1}$	$\nu_{12}$ $\text{mm}^2\cdot\text{s}^{-1}$	$\nu_{21}$ $\text{mm}^2\cdot\text{s}^{-1}$	$\sigma\cdot 10^3$ $\text{mm}^2\cdot\text{s}^{-1}$
293.15	3.24	2.41	8.1	1.77	1.82	2.5
303.15	2.41	2.02	5.6	1.52	1.56	1.6
313.15	2.24	1.71	4.9	1.31	1.34	1.3
323.15	1.88	1.49	4.7	1.16	1.18	1.3
333.15	1.62	1.30	4.3	1.03	1.05	1.1
343.15	1.42	1.15	3.7	0.925	0.932	1.3
353.15	1.26	1.02	2.6	0.832	0.840	1.0
363.15	1.11	0.923	4.2	0.756	0.763	1.0
373.15	1.01	0.832	1.9	0.693	0.699	0.9

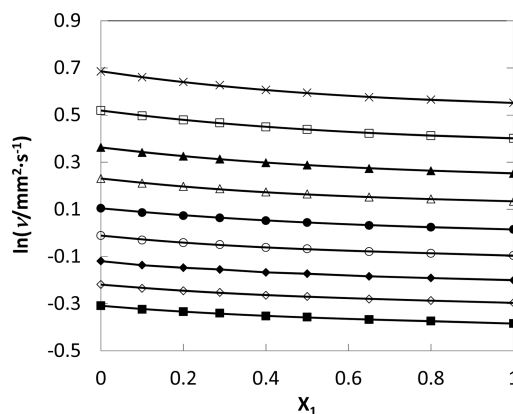


**Figure 4.** Viscosity of 2,2,4,4,6,8,8-heptamethylnonane ( $X_1$ ) + *n*-dodecane mixtures at  $\times$ , 293.15 K;  $\square$ , 303.15 K;  $\blacktriangle$ , 313.15 K;  $\triangle$ , 323.15 K;  $\bullet$ , 333.15 K;  $\circ$ , 343.15 K;  $\blacklozenge$ , 353.15 K;  $\diamond$ , 363.15 K;  $\blacksquare$ , 373.15 K. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ), are smaller than symbols. Lines shown are linear fits to eq 5 with the coefficients in Table 7.

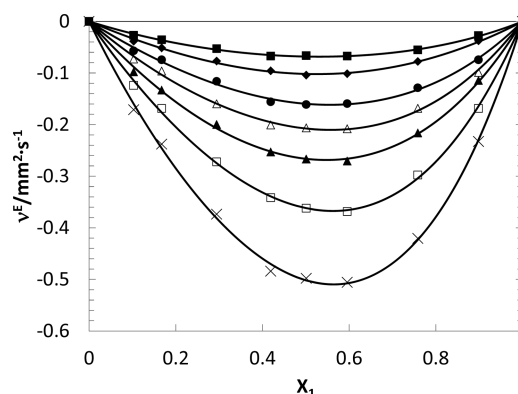
The viscosity deviation ( $\nu^E$ ), sometimes referred to as excess viscosity,<sup>38</sup> in these two-component systems was calculated using:

$$\nu^E = \nu_m - (X_1\nu_1) - (X_2\nu_2) \quad (7)$$

$\nu_m$  is the kinematic viscosity of the binary mixture,  $\nu_1$  and  $\nu_2$  are the kinematic viscosities of the pure components, and  $X_1$  and  $X_2$  are the mole fractions of the branched alkane as component 1 and *n*-dodecane as component 2. The calculated values of the viscosity deviations for all two-component mixtures are given in Tables S1 and S2 of the Supporting Information. Figure 6 shows that the viscosity deviations for mixtures containing 2,2,4,4,6,8,8-heptamethylnonane and *n*-dodecane are small and negative and that the deviations become less negative as temperature increases. For mixtures containing 2,2,4,6,6-pentamethylheptane and *n*-dodecane, the viscosity deviations



**Figure 5.** Viscosity of 2,2,4,6,6-pentamethylheptane ( $X_1$ ) + *n*-dodecane mixtures at  $\times$ , 293.15 K;  $\square$ , 303.15 K;  $\blacktriangle$ , 313.15 K;  $\triangle$ , 323.15 K;  $\bullet$ , 333.15 K;  $\circ$ , 343.15 K;  $\blacklozenge$ , 353.15 K;  $\diamond$ , 363.15 K;  $\blacksquare$ , 373.15 K. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ), are smaller than symbols. Lines shown are linear fits to eq 5 with the coefficients in Table 7.



**Figure 6.** Viscosity deviation of 2,2,4,4,6,8,8-heptamethylnonane ( $X_1$ ) + *n*-dodecane mixtures at as calculated by eq 7: at  $\times$ , 293.15 K;  $\square$ , 303.15 K;  $\blacktriangle$ , 313.15 K;  $\triangle$ , 323.15 K;  $\bullet$ , 333.15 K;  $\circ$ , 343.15 K;  $\blacklozenge$ , 353.15 K;  $\diamond$ , 363.15 K;  $\blacksquare$ , 373.15 K. Lines shown are linear fits to eq 8 with the coefficients in Table 8.

are very small, with the greatest deviation from zero exhibited by the mixture with a mole fraction of 0.4999 at 293.15 K having a viscosity deviation of  $-0.05 \text{ mm}^2\cdot\text{s}^{-1}$ . At 343.15 K and above, the viscosity deviations do not differ from zero when accounting for their error.

The viscosity deviations for the 2,2,4,4,6,8,8-heptamethylnonane and *n*-dodecane mixtures were fit to a Redlich–Kister type expression<sup>32</sup>

$$\ln \nu^E = X_1 X_2 \sum_{j=0}^{j-1} A_j (X_1 - X_2)^j \quad (8)$$

where  $A_j$  are adjustable parameters,  $j$  is the order of the polynomial, and  $X_1$  and  $X_2$  are the mole fractions of 2,2,4,4,6,8,8-heptamethylnonane and *n*-dodecane, respectively. The standard error for the fit ( $\sigma$ ) was determined by eq 2, where  $P_{\text{measured}}$  is the calculated viscosity deviation, and  $P_{\text{fit}}$  is the fitted viscosity deviation. The fitted values of  $A_1$ ,  $A_2$ , and  $A_3$ , and the standard errors of the fits are given in Table 8 for each temperature. The model fits the data well as shown in Figure 6.

The viscosity values for the hydrotreated renewable fuels fall within the viscosity values of the some of the mixtures

**Table 8. Parameters for Redlich–Kister Equation, eq 8, and the Standard Errors for Mixtures of 2,2,4,4,6,8,8-Heptamethylnonane (1) in (2,2,4,4,6,8,8-Heptamethylnonane + *n*-Dodecane) at 0.1 MPa**

<i>T</i> /K	<i>A</i> <sub>1</sub>	<i>A</i> <sub>2</sub>	<i>A</i> <sub>3</sub>	$\sigma \cdot 10^3$
	mm <sup>2</sup> ·s <sup>-1</sup>	mm <sup>2</sup> ·s <sup>-1</sup>	mm <sup>2</sup> ·s <sup>-1</sup>	mm <sup>2</sup> ·s <sup>-1</sup>
293.15	-2.007	-0.491	-0.187	8.2
303.15	-1.447	-0.351	-0.116	5.4
313.15	-1.065	-0.199	-0.085	4.6
323.15	-0.830	-0.183	-0.075	4.8
333.15	-0.639	-0.143	-0.038	4.3
343.15	-0.515	-0.099	-0.0727	3.3
353.15	-0.407	-0.043	0.0132	2.7
363.15	-0.326	-0.055	-0.0548	3.3
373.15	-0.271	-0.033	-0.0314	1.6

measured herein. At 293.15 K, the viscosities of (1.97, 2.74, and 3.40) mPa·s for camelina HRJ-5, DSH-76, and algal HRD-76, respectively, fall within the viscosity values of the mixtures of 2,2,4,4,6,8,8-heptamethylnonane in *n*-dodecane measured herein, (1.49 to 3.70) mPa·s.<sup>7,23,24</sup> The viscosity of tallow HRJ-5, 1.41 mPa·s, falls within the viscosity values for mixtures of 2,2,4,6,6-pentamethylheptane and *n*-dodecane, (1.29 to 1.49) mPa·s, at 293.15 K.<sup>24</sup>

**4.3. Speed of Sound and Bulk Modulus.** The speed of sound values are given in Table 9 for the *n*-dodecane, 2,2,4,4,6,8,8-heptamethylnonane, and their mixtures as a function of the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane and in Table 10 for the *n*-dodecane, 2,2,4,6,6-pentamethylheptane, and their mixtures as a function of the mole fraction of 2,2,4,6,6-pentamethylheptane. As shown in Table 3, the speed of sound measurements for 2,2,4,4,6,8,8-heptamethylnonane and 2,2,4,6,6-pentamethylheptane agree with values taken at the same temperatures using the same instrument.<sup>7,23</sup> The speed of sound measurements for *n*-dodecane fall among the measurements reported previously as shown in Figure 7 and in Table 3. Speed of sound and temperature data were fit to

$$c/\text{m}\cdot\text{s}^{-1} = AT/K + B \quad (9)$$

using the Microsoft Excel linear regression software in its Analysis Toolpak, and the standard error was calculated by eq 2 with speed of sound as parameter *P*. For *n*-dodecane the relationship

$$c/\text{m}\cdot\text{s}^{-1} = -3.75T/K + 2397 \quad (10)$$

fits the data well ( $R^2 = 0.9999$ ) as shown in Figure 7. Other literature values fall on this line. For example at 318.15 K, eq 10

predicts that the speed of sound would be  $1203.2 \pm 0.3 \text{ m}\cdot\text{s}^{-1}$ , which matches the value reported by Abinabhavi and Gopalkrishna,  $1203 \text{ m}\cdot\text{s}^{-1}$ .<sup>43</sup>

The speed of sound of all mixtures decreased as temperature increased (Tables 9 and 10), and the decline was linear over the temperature range measured as shown in Figures 8 and 9. The temperature and speed of sound data for all mixtures were fit to eq 9, with the fitting parameters given in Table 11. All fits are good with  $R^2 \geq 0.9999$  as shown in Figures 8 and 9 for 2,2,4,4,6,8,8-heptamethylnonane and 2,2,4,6,6-pentamethylheptane mixtures, respectively.

The isentropic bulk modulus,  $E_v$ , was calculated at each temperature and ambient pressure from the speed of sound (*c*) and density ( $\rho$ ) by:<sup>45</sup>

$$E_v/\text{Pa} = (c^2/\text{m}^2\cdot\text{s}^{-2})(\rho/\text{kg}\cdot\text{m}^{-3}) \quad (11)$$

These values are given in Tables 12 and 13. The bulk modulus decreases as temperature increases, as the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane in *n*-hexadecane decreases (Table 12), and as the mole fraction of 2,2,4,6,6-pentamethylheptane increases (Table 13).

The speed of sound and isentropic bulk modulus for the hydrotreated renewable fuels are modestly higher or match the values for these mixtures. At 293.15 K, the speed of sound values of  $(1301.0 \pm 0.6, 1308.5 \pm 0.3, \text{ and } 1340.9 \pm 0.6) \text{ m}\cdot\text{s}^{-1}$  for camelina HRJ-5, DSH-76, and algal HRD-76, respectively, exceed the speed of sound measured herein for the 2,2,4,4,6,8,8-heptamethylnonane in *n*-dodecane mixtures ( $1285.7$  to  $1297.6) \text{ m}\cdot\text{s}^{-1}$  and the 2,2,4,6,6-pentamethylheptane in *n*-dodecane mixtures ( $1203.6$  to  $1297.6) \text{ m}\cdot\text{s}^{-1}$ .<sup>7,23,24</sup> Only the tallow HRJ-5 with a speed of sound of  $1279.8 \pm 0.6$  at 293.15 K falls within the range of values for the 2,2,4,6,6-pentamethylheptane in *n*-dodecane mixtures.<sup>24</sup> At 293.15 K, the bulk moduli of  $(1317 \pm 0.3, \text{ and } 1395 \pm 2) \text{ MPa}$  for DSH-76 and algal HRD-76, respectively, exceed the bulk moduli measured herein for the 2,2,4,4,6,8,8-heptamethylnonane in *n*-dodecane mixtures  $[(1261 \text{ to } 1297) \text{ MPa}]$  and the 2,2,4,6,6-pentamethylheptane in *n*-dodecane mixtures  $[(1080 \text{ to } 1261) \text{ MPa}]$ .<sup>7,23</sup> The bulk modulus of  $1234 \pm 1 \text{ MPa}$  for tallow HRJ-5 at 293.15 K falls within the range of values for the 2,2,4,4,6,8,8-heptamethylnonane in *n*-dodecane mixtures, while the bulk modulus of  $1294 \pm 1 \text{ MPa}$  for camelina HRJ-5 falls within the range of values for *n*-dodecane with either branched alkane.<sup>24</sup>

**4.4. Flash Point and Surface Tension.** The surface tension and flash point values are given in Table 14 for the mixtures studied herein as a function of the mole fraction of the branched alkane. The surface tension values of *n*-dodecane are shown with literature values in Figure 10.<sup>46–48</sup> A linear regression of surface tension versus temperature data found in

**Table 9. Experimental Values of Speed of Sound *c* (m·s<sup>-1</sup>) of Mixtures of 2,2,4,4,6,8,8-Heptamethylnonane (1) + *n*-Dodecane from *T* = (293 to 333) K and 0.1 MPa<sup>a</sup>**

<i>T</i> /K	<i>X</i> <sub>1</sub>									
	0.0000	0.1030	0.1677	0.2944	0.4191	0.5011	0.5955	0.7585	0.8985	1.0000
293.15	1297.6	1295.6	1294.1	1292.0	1290.5	1289.5	1288.5	1287.2	1286.3	1285.7
303.15	1259.3	1257.5	1256.2	1254.3	1252.9	1252.0	1251.0	1249.8	1248.9	1248.5
313.15	1221.4	1219.8	1218.7	1217.0	1215.7	1214.9	1214.1	1213.0	1212.2	1211.8
323.15	1184.2	1182.8	1181.8	1180.3	1179.2	1178.5	1177.8	1176.8	1176.3	1176.0
333.15	1147.5	1146.3	1145.4	1144.2	1143.3	1142.7	1142.2	1141.4	1141.0	1140.8

<sup>a</sup>*X*<sub>1</sub> is the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane in the (2,2,4,4,6,8,8-heptamethylnonane + *n*-dodecane) mixture. The standard uncertainty *u* is *u*(*T*) = 0.01 K, and the combined expanded uncertainty *U*<sub>*c*</sub> is *U*<sub>*c*</sub>(*c*) = 0.3 m·s<sup>-1</sup>.



Table 10. Experimental Values of Speed of Sound  $c$  ( $\text{m}\cdot\text{s}^{-1}$ ) of Mixtures of 2,2,4,6,6-Pentamethylheptane (1) +  $n$ -Dodecane from  $T = (293 \text{ to } 333) \text{ K}$  and  $0.1 \text{ MPa}$ <sup>a</sup>

$T/\text{K}$	$X_1$								
	0.0000	0.1000	0.2000	0.2885	0.3998	0.4999	0.6501	0.7998	1.0000
293.15	1297.6	1288.5	1279.3	1271.4	1261.4	1251.6	1238.0	1223.2	1203.6
303.15	1259.3	1250.3	1241.1	1233.2	1223.2	1213.4	1199.6	1184.7	1164.8
313.15	1221.4	1212.5	1203.3	1195.5	1185.4	1175.7	1161.8	1146.8	1126.7
323.15	1184.2	1175.3	1166.2	1158.3	1148.3	1138.5	1124.6	1109.5	1089.3
333.15	1147.5	1138.7	1129.6	1121.7	1111.7	1101.9	1087.9	1072.8	1052.5

<sup>a</sup> $X_1$  is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane +  $n$ -dodecane) mixture. The standard uncertainty  $u$  is  $u(T) = 0.01 \text{ K}$ , and the combined expanded uncertainty  $U_c$  is  $U_c(c) = 0.3 \text{ m}\cdot\text{s}^{-1}$ .

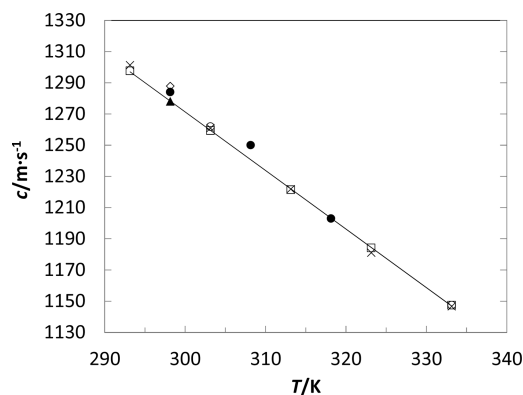


Figure 7. Speed of sound of  $n$ -dodecane:  $\square$ , this study;  $\times$ , ref 36;  $\diamond$ , ref 38;  $\circ$ , ref 42;  $\bullet$ , ref 43;  $\blacktriangle$ , ref 44. The line shown is a linear fit, eq 10.

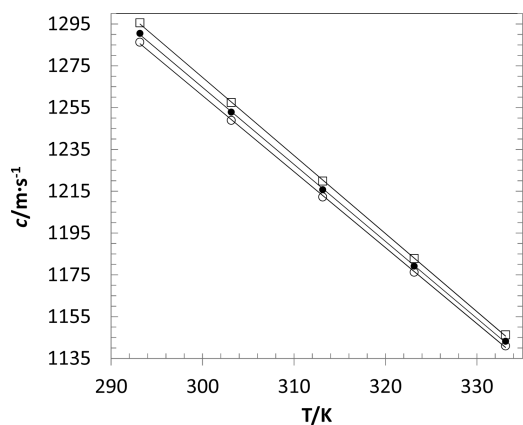


Figure 8. Speed of sound of 2,2,4,4,6,8,8-heptamethylnonane ( $X_1$ ) +  $n$ -dodecane mixtures at mole fractions:  $\square$ ,  $X_1 = 0.1030$ ;  $\bullet$ ,  $X_1 = 0.4191$ ;  $\circ$ ,  $X_1 = 0.8985$ . Error bars, which are the combined expanded uncertainties with 0.95 level of confidence ( $k \approx 2$ ), are smaller than symbols. Lines shown are linear fits using eq 9 with the coefficients in Table 11.

the Jasper and Kring<sup>46</sup> for  $n$ -dodecane (Figure 10) predicts that the value of surface tension at  $294.7 \text{ K}$  should be  $25.2 \text{ mN}\cdot\text{m}^{-1}$ , which agrees with the data reported herein of  $25.3 \pm 0.2 \text{ mN}\cdot\text{m}^{-1}$ . The surface tension for 2,2,4,4,6,8,8-heptamethylnonane,  $24.0 \pm 0.2 \text{ mN}\cdot\text{m}^{-1}$ , agrees with the data reported previously using the same instrument,  $24.1 \pm 0.2 \text{ mN}\cdot\text{m}^{-1}$ , but with samples from different manufacturer lots (Table 3).<sup>7</sup> The surface tension for 2,2,4,6,6-pentamethylheptane was taken from Luning Prak et al.<sup>23</sup> As can be seen in Figure 11, the surface tension decreases as the mole fraction of the branched component increases, but the trend is not linear.

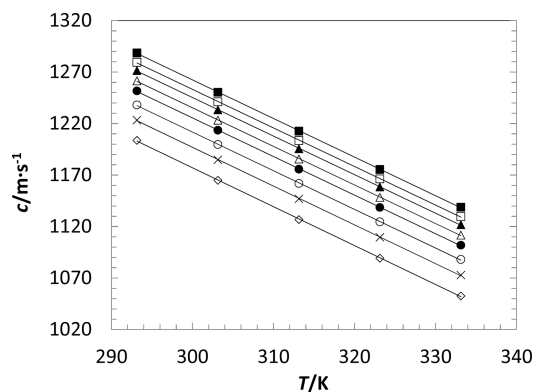


Figure 9. Speed of sound of 2,2,4,6,6-pentamethylheptane ( $X_1$ ) +  $n$ -dodecane mixtures at mole fractions:  $\blacksquare$ ,  $X_1 = 0.1000$ ;  $\square$ ,  $X_1 = 0.2000$ ;  $\blacktriangle$ ,  $X_1 = 0.2885$ ;  $\triangle$ ,  $X_1 = 0.3998$ ;  $\bullet$ ,  $X_1 = 0.4999$ ;  $\circ$ ,  $X_1 = 0.6501$ ;  $\times$ ,  $X_1 = 0.7998$ ;  $\diamond$ ,  $X_1 = 1.000$ . Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ), are smaller than symbols. Lines shown are linear fits using eq 9 with the coefficients in Table 11.

For flash point, increasing the concentration of 2,2,4,4,6,8,8-heptamethylnonane in  $n$ -dodecane increases the flash point, while the trend is opposite for 2,2,4,6,6-pentamethylheptane (Table 14). These trends are not linear as shown in Figure 12. The flash point of  $354 \pm 2 \text{ K}$  for dodecane falls between the reported values of  $352 \text{ K}$ <sup>49</sup> and  $358 \pm 2 \text{ K}$  (Table 3).<sup>50</sup> The flash points of 2,2,4,4,6,8,8-heptamethylnonane and 2,2,4,6,6-pentamethylheptane were taken from Luning Prak et al.<sup>7,23</sup>

The surface tension and flash point for some of the hydrotreated renewable fuels are matched by values in these mixtures. The surface tensions of  $(23.1, 23.9, \text{ and } 25.0) \text{ mN}\cdot\text{m}^{-1}$  for tallow HRJ-5,<sup>51</sup> camelina HRJ-5,<sup>52</sup> and DSH-76,<sup>23</sup> respectively, fall within the surface tensions measured herein for either the 2,2,4,4,6,8,8-heptamethylnonane in  $n$ -dodecane mixtures ( $24.0 \text{ to } 25.3) \text{ mN}\cdot\text{m}^{-2}$  or the 2,2,4,6,6-pentamethylheptane in  $n$ -dodecane mixtures ( $21.8 \text{ to } 25.3) \text{ mN}\cdot\text{m}^{-1}$ . The surface tension of algal HRD-76,  $26.0 \text{ mN}\cdot\text{m}^{-1}$ ,<sup>7</sup> exceeds the surface tensions measured herein. The flash point values of  $(360 \text{ and } 378) \text{ K}$  for algal HRD-76<sup>7</sup> and DSH-76,<sup>23</sup> respectively, exceed the flash point measured herein for the 2,2,4,4,6,8,8-heptamethylnonane in  $n$ -dodecane mixtures,  $(354 \text{ to } 357) \text{ K}$ , and for the 2,2,4,6,6-pentamethylheptane in  $n$ -dodecane mixtures,  $(318 \text{ to } 354) \text{ K}$ . The flash point of the HRJ-5 camelina,  $335 \text{ K}$ ,<sup>52</sup> falls with the range of values for the 2,2,4,6,6-pentamethylheptane in  $n$ -dodecane mixtures.

Table 11. Parameters for eq 10:  $c = AT/K + B$ , That Relates Speed of Sound,  $c$  ( $m \cdot s^{-1}$ ), to Temperature for 2,2,4,4,6,8,8-Heptamethylnonane (1) in (2,2,4,4,6,8,8-Heptamethylnonane + *n*-Dodecane) Mixtures and for 2,2,4,6,6-Pentamethylheptane (2) in the (2,2,4,6,6-Pentamethylheptane + *n*-Dodecane) Mixtures over the Temperature Range  $T = (293 \text{ to } 333) \text{ K}$  and the Standard Errors<sup>a</sup>

2,2,4,4,6,8,8-heptamethylnonane mixtures					2,2,4,6,6-pentamethylheptane mixtures				
$X_1$	$A/K^{-1}$	$B/m \cdot s^{-1}$	$R^2$	$\sigma$	$X_2$	$A/K^{-1}$	$B/m \cdot s^{-1}$	$R^2$	$\sigma$
0.0000	$-3.75 \pm 0.06$	$2397 \pm 19$	0.9999	1.3	0.0000	$-3.75 \pm 0.06$	$2397 \pm 19$	0.9999	1.3
0.1030	$-3.73 \pm 0.06$	$2389 \pm 19$	0.9999	1.3	0.1000	$-3.75 \pm 0.06$	$2386 \pm 19$	0.9999	1.3
0.1677	$-3.72 \pm 0.06$	$2384 \pm 19$	0.9999	1.3	0.2000	$-3.74 \pm 0.06$	$2376 \pm 19$	0.9999	1.3
0.2944	$-3.70 \pm 0.06$	$2375 \pm 19$	0.9999	1.4	0.2885	$-3.74 \pm 0.06$	$2369 \pm 19$	0.9999	1.3
0.4191	$-3.68 \pm 0.06$	$2369 \pm 20$	0.9999	1.4	0.3998	$-3.75 \pm 0.06$	$2359 \pm 19$	0.9999	1.4
0.5011	$-3.67 \pm 0.07$	$2365 \pm 21$	0.9999	1.5	0.4999	$-3.75 \pm 0.06$	$2349 \pm 19$	0.9999	1.4
0.5955	$-3.66 \pm 0.07$	$2361 \pm 22$	0.9999	1.5	0.6501	$-3.75 \pm 0.06$	$2337 \pm 20$	0.9999	1.4
0.7585	$-3.65 \pm 0.07$	$2355 \pm 22$	0.9999	1.5	0.7998	$-3.76 \pm 0.07$	$2325 \pm 21$	0.9999	1.5
0.8985	$-3.63 \pm 0.08$	$2351 \pm 24$	0.9998	1.7	1.0000	$-3.78 \pm 0.08$	$2310 \pm 24$	0.9998	1.7
1.0000	$-3.62 \pm 0.08$	$2347 \pm 24$	0.9998	1.7					

<sup>a</sup>Error bars are the 95 % confidence interval.

Table 12. Calculated Isentropic Bulk Modulus (MPa) of Mixtures of 2,2,4,4,6,8,8-Heptamethylnonane (1) + *n*-Dodecane from  $T = (293 \text{ to } 333) \text{ K}$  and 0.1 MPa<sup>a</sup>

$T/K$	$X_1$									
	0.0000	0.1030	0.1677	0.2944	0.4191	0.5011	0.5955	0.7585	0.8985	1.0000
293.15	1261	1264	1266	1270	1275	1278	1281	1288	1293	1297
303.15	1176	1180	1182	1186	1191	1194	1197	1203	1209	1212
313.15	1096	1099	1102	1106	1111	1114	1117	1123	1129	1132
323.15	1020	1024	1026	1031	1035	1039	1042	1048	1053	1057
333.15	948	952	955	959	964	967	971	977	982	986

<sup>a</sup> $X_1$  is the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane in the (2,2,4,4,6,8,8-heptamethylnonane + *n*-dodecane) mixture. The standard uncertainty  $u$  is  $u(T) = 0.01 \text{ K}$ , and the combined expanded uncertainty  $U(E_v)$  is  $U_c(E_v) = 0.4 \text{ MPa}$ .

Table 13. Calculated Isentropic Bulk Modulus (MPa) of Mixtures of 2,2,4,6,6-Pentamethylheptane (1) + *n*-Dodecane from  $T = (293 \text{ to } 333) \text{ K}$  and 0.1 MPa<sup>a</sup>

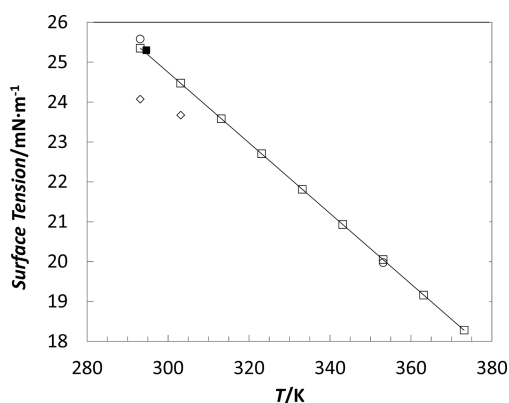
T/K	$X_1$								
	0.0000	0.1000	0.2000	0.2885	0.3998	0.4999	0.6501	0.7998	1.0000
293.15	1261	1243	1224	1209	1189	1170	1144	1116	1080
303.15	1176	1159	1141	1126	1107	1089	1064	1037	1001
313.15	1096	1079	1062	1048	1030	1013	988	962	927
323.15	1020	1004	988	974	957	940	917	891	858
333.15	948	933	918	904	888	872	849	825	793

<sup>a</sup> $X_1$  is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + *n*-dodecane) mixture. The standard uncertainty  $u$  is  $u(T) = 0.01 \text{ K}$ , and the combined expanded uncertainty  $U(E_v)$  is  $U_c(E_v) = 0.4 \text{ MPa}$ .

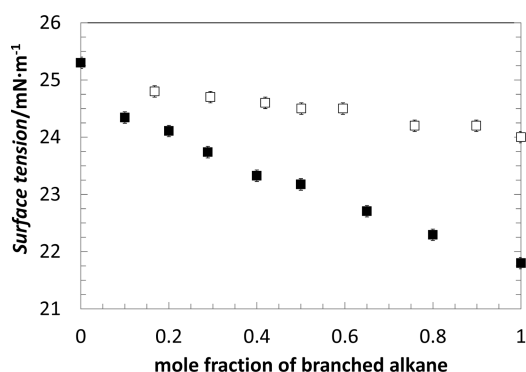
Table 14. Experimental Values of Flash Point and Surface Tension of 2,2,4,4,6,8,8-Heptamethylnonane (1) + *n*-Dodecane Mixtures and 2,2,4,6,6-Pentamethylheptane (2) + *n*-Dodecane Mixtures<sup>a</sup>

	$X_1$								
	0.0000	0.1677	0.2944	0.4191	0.5011	0.5955	0.7585	0.8985	1.0000
flash point/K	354	355	357	358	359	360	363	365	367
surface tension/mN·m <sup>-1</sup>	25.3	24.8	24.9	24.6	24.6	24.3	24.2	24.2	24.0
	$X_2$								
	0.0000	0.1000	0.2000	0.2885	0.3998	0.4999	0.6501	0.7998	1.0000
flash point/K	354	346	340	337	332	329	325	322	318 <sup>b</sup>
surface tension/mN·m <sup>-1</sup>	25.3	24.3	24.1	23.7	23.3	23.2	22.7	22.3	21.8 <sup>b</sup>

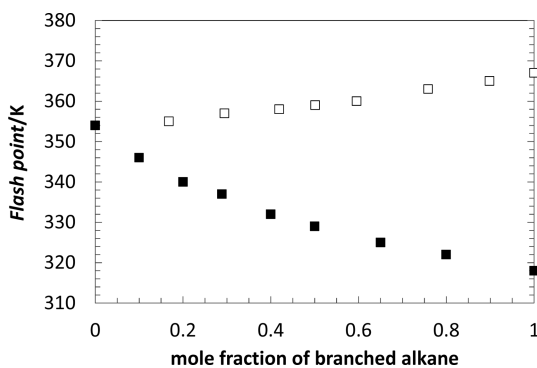
<sup>a</sup> $X_1$  is the mole fraction of 2,2,4,4,6,8,8-heptamethylnonane in the (2,2,4,4,6,8,8-heptamethylnonane + *n*-dodecane) mixture, and  $X_2$  is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + *n*-dodecane) mixtures. Combined expanded uncertainties  $U_c$  are  $U(X_1) \leq 0.0001$ ,  $U_c(\text{flash point}) = 2 \text{ K}$ , and  $U_c(\text{surface tension}) = 0.2 \text{ mN} \cdot \text{m}^{-2}$  (level of confidence = 0.95,  $k \approx 2$ ). Surface tension measurements were taken at room temperature,  $294.7 \pm 1 \text{ K}$ . <sup>b</sup>Taken from ref 23.



**Figure 10.** Surface tension of dodecane: ■, this study; □, ref 46; ○, ref 47; ◇, ref 48. The error bars, which are the combined expanded uncertainties with 0.95 level of confidence ( $k \approx 2$ ), are smaller than symbols. The line is a regression of the data found in Jasper and Kring.<sup>46</sup>



**Figure 11.** Surface tension of mixtures: ■, 2,2,4,6,6-pentamethylheptane + *n*-dodecane and □, 2,2,4,4,6,8,8-heptamethylnonane + *n*-dodecane. The error bars are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ).



**Figure 12.** Flash point of mixtures: ■, 2,2,4,6,6-pentamethylheptane + *n*-dodecane and □, 2,2,4,4,6,8,8-heptamethylnonane + *n*-dodecane. The error bars are the combined expanded uncertainties with a 0.95 level of confidence ( $k \approx 2$ ).

## 5. CONCLUSION

In this work, the physical properties *n*-dodecane with 2,2,4,6,6-pentamethylheptane or 2,2,4,4,6,8,8-heptamethylnonane were measured and compared to properties of hydrotreated diesel fuels, algal HRD-76 and DSH-76, and hydrotreated jet fuels, camelina HRJ-5 and tallow HRJ-5. Many of the pure component measurements of the pure components fell within values reported in the literature. The densities of the mixtures

were well-modeled using a second-order polynomial function, and the viscosity was well-modeled using the McAllister three-body model. A linear relationship was found between the speed of sound and temperature. Neither flash point nor surface tension were linearly related to mole fraction of the branched alkane. The comparison of the mixture data with values reported for hydrotreated fuel showed that some of properties of the fuels fell within the range of the mixtures, and the match was better for the jet fuels than for the diesel fuels. For the diesel algal HRD-76, the density and viscosity were matched by mixtures of *n*-dodecane with 2,2,4,4,6,8,8-heptamethylnonane, but speed of sound, bulk modulus, surface tension and flash point were higher than values for all mixtures. For the diesel DSH-76, the density, viscosity, and surface tension were matched by mixtures of *n*-dodecane with 2,2,4,4,6,8,8-heptamethylnonane, but speed of sound, bulk modulus, and flash point were higher than values for all mixtures. For the jet fuel camelina HRJ-5, the density, viscosity, bulk modulus, and surface tension were matched by mixtures of *n*-dodecane with 2,2,4,4,6,8,8-heptamethylnonane, while only the speed of sound was higher than values for all mixtures. For the jet fuel tallow HRJ-5, the density, viscosity, speed of sound, bulk modulus, surface tension, and flash point were matched by mixtures of *n*-dodecane with 2,2,4,6,6-pentamethylheptane.

These data suggest that binary mixtures of *n*-dodecane with branched alkanes may be suitable surrogates for some hydrotreated renewable fuels.

## ■ ASSOCIATED CONTENT

### Supporting Information

Values of the viscosity deviations  $\eta^E$  for the mixtures. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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