

COMPONENTS:		EVALUATOR:	
(1) 2-Heptene; C <sub>7</sub> H <sub>14</sub> ; [592-77-8]		G.T. Hefter	
(2) Water; H <sub>2</sub> O; [7732-18-5]		School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia.	
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CRITICAL EVALUATION:			
Quantitative data for the solubility of 2-heptene (1) in water (2) have been reported in the publications listed in Table 1.			
<u>TABLE 1: Quantitative Solubility Studies of 2-Heptene (1) in Water (2)</u>			
Reference	T/K	Method	Solubility values <sup>a</sup> 10 <sup>3</sup> g(1)/100g sln    10 <sup>6</sup> x <sub>1</sub>
McAuliffe (ref 1)	298	GLC	15 (R)    2.7 (R)
Schwarz (ref 2)	297	chromatographic	15 (R)    2.7 (R)
<p><sup>a</sup> (R) - Recommended value</p> <p>The agreement between the two studies is excellent and although the measurement temperatures differ slightly this effect should be minor. The values in Table 1 are therefore Recommended.</p> <p>Solubility values of 2-heptene in various salt solutions have also been reported (ref 3) but, although in broad agreement with the values given in Table 1 will not be considered in this Evaluation. No data are available for the solubility of water in 2-heptene.</p>			
REFERENCES			
1. McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75.			
2. Schwarz, F.P. <i>Anal. Chem.</i> <u>1980</u> , <i>52</i> , 10-15.			
3. Natarajan, G.S.; Venkatachalam, K.A. <i>J. Chem. Eng. Data</i> <u>1972</u> , <i>17</i> , 328-9.			

<b>COMPONENTS:</b>  (1) 2-Heptene; C <sub>7</sub> H <sub>14</sub> ; [592-77-8]  (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  McAuliffe, C.  <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  A. Maczynski, Z. Maczynska, and A. Szafranski
<b>EXPERIMENTAL VALUES:</b>  The solubility of 2-heptene in water at 25°C was reported to be 15 g(1)/10 <sup>6</sup> g(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 0.0015 g(1)/100 g sln and $2.7 \times 10^{-6}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/Apparatus/Procedure:</b>  In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Phillips Petroleum or Columbia Chemical; used as received.  (2) distilled.  <b>ESTIMATED ERROR:</b> temp. ± 1.5 K soly. 1.4 g(1)/10 <sup>6</sup> g(2) (standard deviation of mean)  <b>REFERENCES:</b>

<b>COMPONENTS:</b>  (1) 2-Heptene; $C_7H_{14}$ ; [592-77-8] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Schwarz, F.P. <i>Anal. Chem.</i> <u>1980</u> , 52, 10-15.
<b>VARIABLES:</b>  One temperature: 23.5°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b>  Solubility of 2-heptene in water at 23.5°C was reported to be $0.00150 \pm 0.00003$ g(l)/100 g sln. The corresponding mole fraction, $x_1$ , calculated by the compiler is $2.75 \times 10^{-6}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b> An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) 99% purity used without further purification (2) distilled  <b>ESTIMATED ERROR:</b> temp. $\pm 1.5^\circ C$ soly. 2% (average std. dev.)  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) 2-Heptene; C <sub>7</sub> H <sub>14</sub> ; [592-77-8] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Natarajan, G.S.; Venkatachalam, K.A. <i>J. Chem. Eng. Data</i> <u>1972</u> , 17, 328-9
<b>VARIABLES:</b> One temperature: 25°C	<b>PREPARED BY:</b> M.C. Haulait-Pirson, G.T. Hefter
<b>EXPERIMENTAL VALUES:</b> <p>The solubility of 2-heptene in water was reported to be <math>2.716 \times 10^{-4}</math> mol L<sup>-1</sup> at 25°C.<sup>a</sup> Assuming a solution density of 1.00 g mL<sup>-1</sup> the corresponding mass percent and mole fraction (<math>x_1</math>) solubilities, calculated by the compilers are respectively, 0.00266 g(l)/100 g sln and <math>4.89 \times 10^{-6}</math>.</p> <p>Solubility data are also presented as a function of temperature in various salt solutions.</p> <p><sup>a</sup> It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol L<sup>-1</sup> HNO<sub>3</sub> solution.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b> 15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostated glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) Prepared by dehydration of 2-heptanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography. (2) Not specified  <b>ESTIMATED ERROR:</b> Temp. ± 0.05 K Soly. not specified  <b>REFERENCES:</b>