

Supporting Information for:

Solubilities and Self-diffusion Coefficients of Light n-alkanes in NaCl  
Solutions at the temperature range (278.15 – 308.15) K and pressure  
range (1 – 300) bar and Thermodynamics Properties of Their  
Corresponding Hydrates at (150 – 290) K and (1 – 7000) bar

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Table S1. Non-bonded parameters for the TIP4P/2005<sup>1</sup> water force field, methane-methane, and methane-water interactions optimized by Docherty.<sup>2</sup>  $\sigma$  and  $\varepsilon$  are the Lennard-Jones parameters, in unit of Å and K, respectively;  $q$  is the partial charge of an atom in units of elementary charge ( $e$ );  $r$  is the distance between particles in units of Å

Model	$\varepsilon/k_B$ (K)	$\sigma$ (Å)	$q_H$ ( $e$ )	$r_{OM}$ (Å)	$r_{OH}$ (Å)	$\angle HOH$ , deg
<b>Water TIP4P/2005</b>	93.2	3.1589	0.5564	0.1546	0.9572	104.52
<b>CH4</b>	147.5	3.73				
<b>Water-CH4 (<math>k_{ij}=1.07</math>)</b>	125.45	3.4445				

Table S2. Non-bonded parameters for the TraPPE<sup>3</sup> alkane force field, and Madrid-2019 ion forcefield.<sup>4</sup>  $\sigma$  and  $\varepsilon$  are the Lennard-Jones parameters, in unit of Å and K, respectively;  $q$  is the partial charge of an atom in units of elementary charge ( $e$ ).

Pseudo (atom)	$\varepsilon/k_B$ (K)	$\sigma$ (Å)	$q_H$ ( $e$ )	Force field
<b>CH3</b>	98	3.75		TraPPE
<b>CH2</b>	46	3.95		
<b>Na<sup>+</sup></b>	177.1257	2.21737	0.85	Madrid-2019
<b>Cl<sup>-</sup></b>	9.256	4.69906	-0.85	
<b>Na<sup>+</sup>-Cl<sup>-</sup></b>	173.142	3.00512		
<b>Na<sup>+</sup>-water</b>	95.4683	2.60838		
<b>Cl<sup>-</sup>-water</b>	7.4584	4.23867		

Table S3. Bonded parameters for the TraPPE<sup>3</sup> alkane force field. Fixed bond lengths are used; The bond-bending energy is calculated according to:  $U_{bend}(\theta) = \frac{k_\theta}{2}(\theta - \theta_{eq})^2$ , where  $k_\theta$  is the force constant,  $\theta$  and  $\theta_{eq}$  are the angle and the equilibrium angle, respectively; The torsion energy is calculated as:  $U_{torsion}(\phi) = c_0 + c_1[1 + \cos(\phi)] + c_2[1 - \cos(2\phi)] + c_3[1 + \cos(3\phi)]$ , where  $c_0$ ,  $c_1$ ,  $c_2$ ,  $c_3$  are constants;  $\phi$  represents the dihedral angle, which corresponds to synperiplanar (*cis*) conformations when  $\phi=0^\circ$ , and antiperiplanar (*trans*) conformations when  $\phi=180^\circ$ .

<b>Bond-stretching interaction</b>				
Type	$r$ (Å)			
<b>CH3-CH3</b>	1.54			
<b>CH3-CH2</b>	1.54			
<b>Bond-bending interaction</b>				
Type	$\theta_{eq}$ (deg)	$k_\theta/k_B$ (K/rad <sup>2</sup> )		
<b>CH3-CH2-CH3</b>	114	62500		
<b>CH3-CH2-CH2</b>	114	62500		
<b>Dihedral torsion parameter</b>				
Type	$c_0/k_B$ (K)	$c_1/k_B$ (K)	$c_2/k_B$ (K)	$c_3/k_B$ (K)
<b>CH3-CH2-CH2-CH3</b>	0.00	355.03	-68.19	791.32

Table S4. Fugacity coefficients obtained by REFPROP<sup>5</sup> for the four light alkanes at different temperatures and pressures

$T$ (K) \ $P$ (bar)	100 bar	phase	200 bar	phase	300 bar	phase
<b>Methane</b>						
278.15	0.80660	G	0.68713	G	0.63856	G
288.15	0.82922	G	0.72169	G	0.67625	G
298.15	0.84912	G	0.75297	G	0.71128	G
308.15	0.86672	G	0.78123	G	0.74371	G
<b>Ethane</b>						
278.15	0.25544	L	0.17176	L	0.15184	L
288.15	0.30216	L	0.20323	L	0.17925	L
298.15	0.35124	L	0.23667	L	0.20841	L
308.15	0.40173	G	0.27168	G	0.23904	G
<b>Propane</b>						
278.15	0.069011	L	0.048906	L	0.045842	L
288.15	0.088635	L	0.062493	L	0.058231	L
298.15	0.11135	L	0.078173	L	0.07246	L
308.15	0.13715	L	0.095941	L	0.08852	L
<b>n-butane</b>						
278.15	0.017921	L	0.0135	L	0.013472	L
288.15	0.024859	L	0.018576	L	0.01838	L
298.15	0.033547	L	0.024887	L	0.024434	L
308.15	0.04417	L	0.032556	L	0.031738	L

$P$  is pressure;  $T$  is temperature; G represents gas phase; L represent liquid phase.

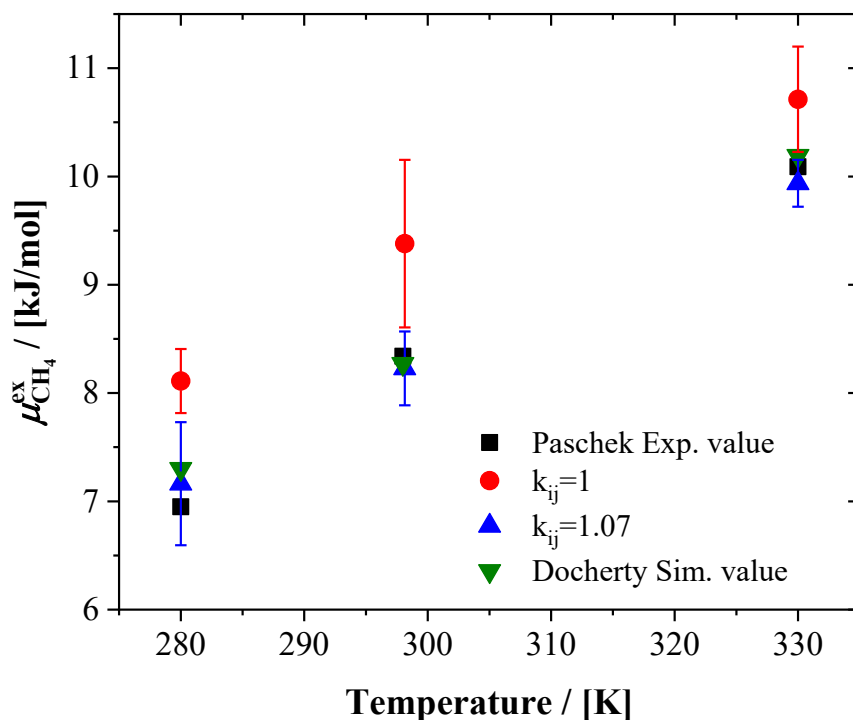


Figure S1. Excess chemical potential of  $\text{CH}_4$  in water at 1 bar as a function of temperature. Docherty's simulation data and Paschek's experimental data are obtained from Ref. [2]<sup>2</sup> and Ref. [6]<sup>6</sup> respectively.

Table S5. Calculated excess chemical potential  $\mu_{ex}$  for ethane in water at 298.15 K and 1 bar using different force field combinations. The reference value from experimental data is equal to 7.59 kJ/mol<sup>7</sup>

Water model	$\text{C}_2\text{H}_6$ model	simulation value	difference
TIP4P2005 <sup>1</sup>	TraPPE <sup>3</sup>	8.38±0.49	0.79
TIP4P2005 <sup>1</sup>	HH-alkane <sup>8</sup>	7.04±0.067	-0.55
TIP4P2005 <sup>1</sup>	NERE <sup>9</sup>	9.02±0.2	1.43
SPC/E <sup>10</sup>	TraPPE <sup>3</sup>	8.51±0.40	0.92
SPC/E <sup>10</sup>	NERE <sup>9</sup>	8.42±0.28	0.83
SPC <sup>11</sup>	TraPPE <sup>3</sup>	8.21±0.28	0.62
SPC <sup>11</sup>	NERE-0.035 <sup>12</sup>	19.45±0.08	11.86
SPC <sup>11</sup>	NERE-0.083 <sup>12</sup>	7.14±0.04	-0.45

Table S6. Calculated excess chemical potential  $\mu_{ex}$  for propane in water at 298.15 K and 1 bar using different force fields for propane

Exp. value <sup>7</sup>	TraPPE <sup>3</sup>	HH-alkane <sup>8</sup>	NERE <sup>9</sup>
8.15	9.5±0.64	8.88±1.14	9.34

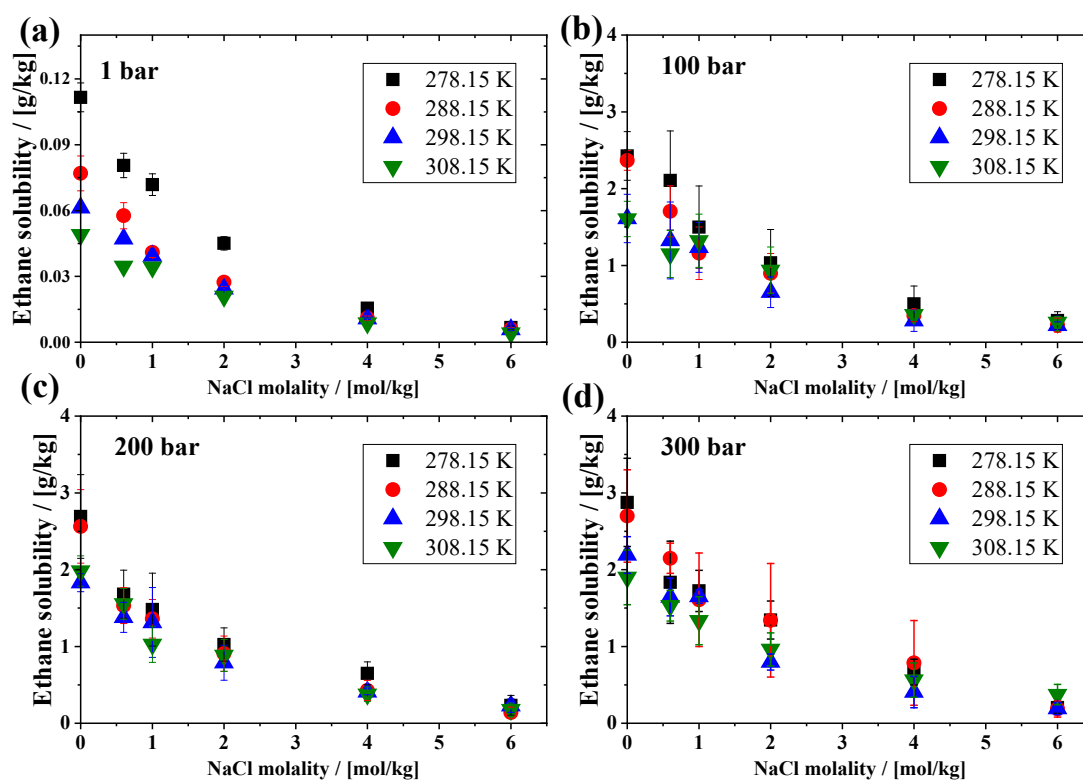


Figure S2. Solubilities of ethane in aqueous NaCl solutions as a function of the NaCl molality at different pressures ((a)1bar, (b)100 bar, (c) 200 bar, (d) 300bar) and temperatures (278.15-308.15 K).

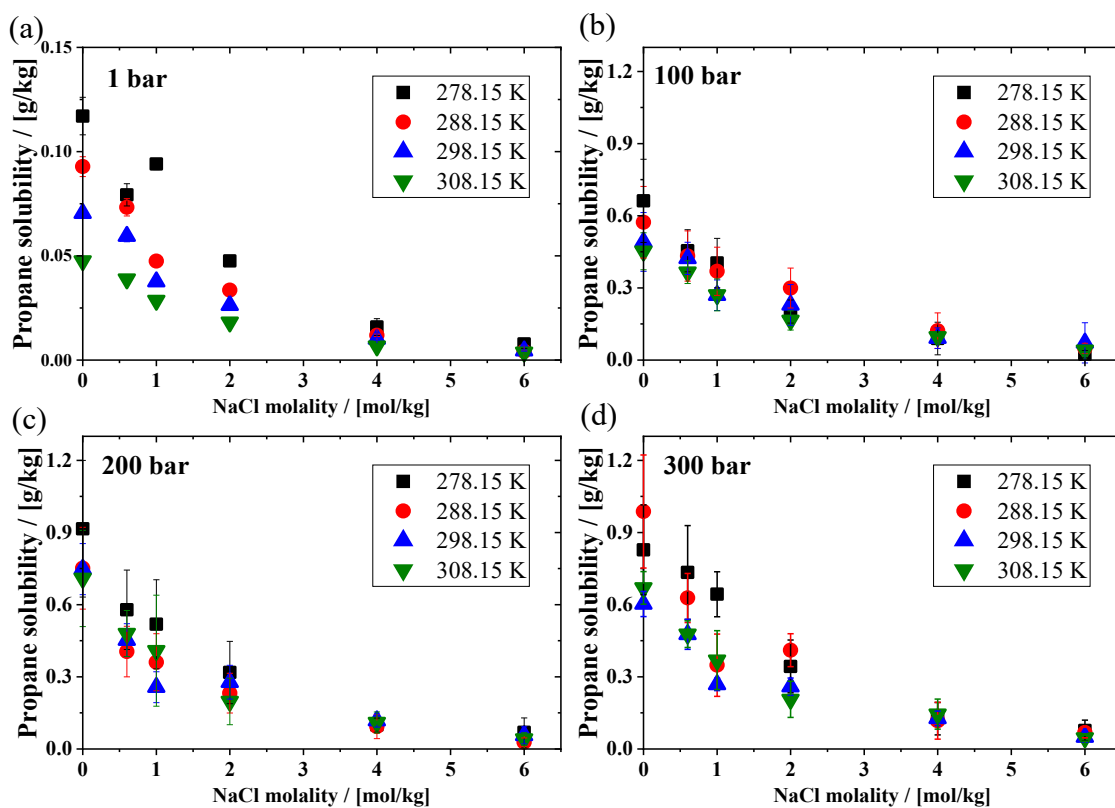


Figure S3. Solubilities of propane in aqueous NaCl solutions as a function of the NaCl molality at different pressures ((a)1bar, (b)100 bar, (c) 200 bar, (d) 300bar) and temperatures (278.15-308.15 K).

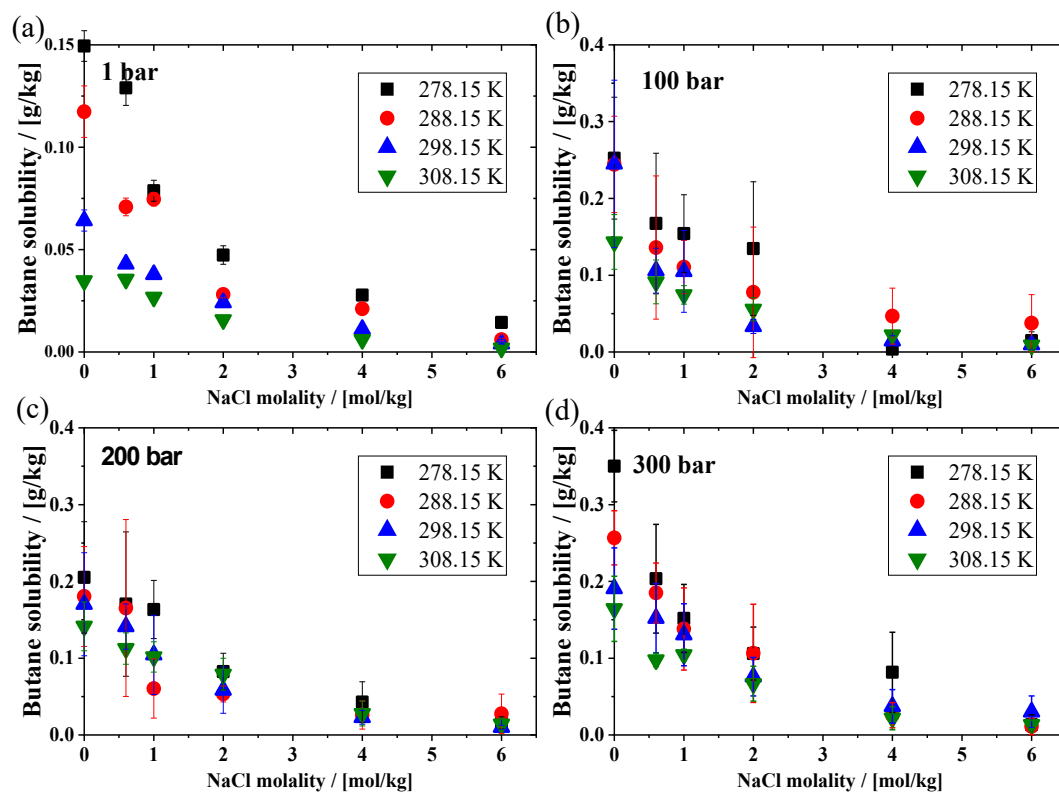


Figure S4. Solubilities of butane in aqueous NaCl solutions as a function of the NaCl molality at different pressures ((a)1bar, (b)100 bar, (c) 200 bar, (d) 300bar) and temperatures (278.15-308.15) K.



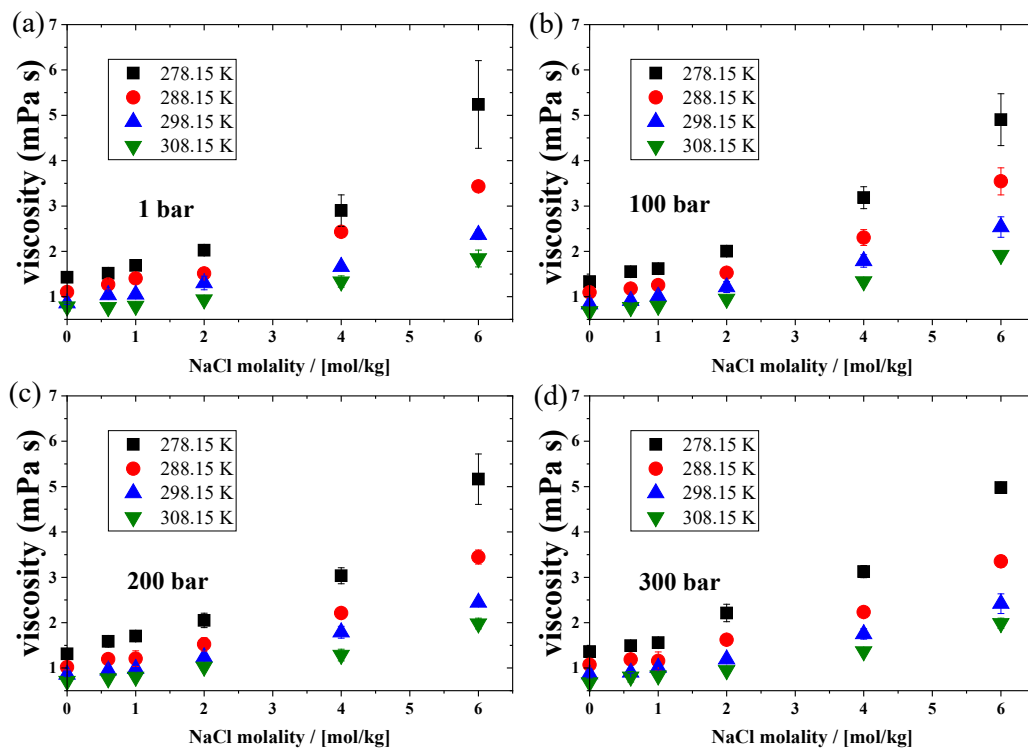


Figure S5. Calculated viscosities of aqueous NaCl solutions with one methane molecule at different temperatures and pressures ((a) 1 bar, (b) 100 bar, (c) 200 bar, (d) 300 bar) as a function of the NaCl molality.

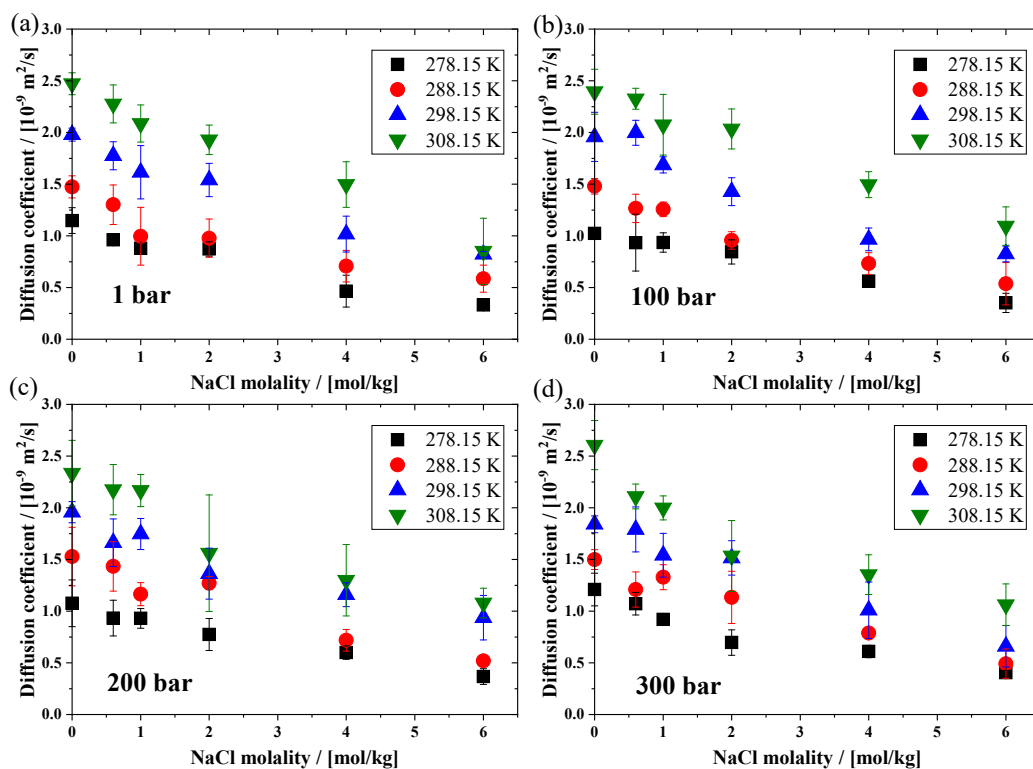


Figure S6. Calculated self-diffusion coefficients of methane in aqueous NaCl solutions at different temperatures and pressures ((a) 1 bar, (b) 100 bar, (c) 200 bar, (d) 300 bar) as a function of NaCl molality.

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