

Sheet1

Unmodified epsilons and sigmas

	Experimental (Pubchem & Mobley DB)	Calculated
density	<b>0.9371</b>	<b>0.95</b>
deltaH	<b>14.1969</b>	<b>13.82</b>
deltaG	<b>-10</b>	<b>-7.09</b>
		Cazade & Bereau & Meuwly
		<b>0.9</b>
		<b>13.76</b>
		<b>-7.34 +/- 0.40</b>

Scaled epsilons and sigmas

	Epsilon*1.05   sigma*1.05	Epsilon*1.1   sigma*1.1
density	<b>0.883</b>	<b>0.805</b>
deltaH	<b>13.569</b>	<b>13.469</b>
deltaG	<b>-6.21</b>	<b>-5.67</b>
	Cazade & Bereau & Meuwly	Cazade & Bereau & Meuwly
density	<b>0.87</b>	<b>0.83</b>
deltaH	<b>13.28</b>	<b>12.77</b>
deltaG	<b>-6.14 +/- 0.14</b>	<b>-5.43 +/- 0.41</b>

	Epsilon*1.025   sigma*1.025	Epsilon*1.075   sigma*1.075
density	<b>0.915</b>	<b>0.843</b>
deltaH	<b>13.68</b>	<b>13.29</b>
deltaG	<b>-6.37</b>	<b>-5.68</b>
	Cazade & Bereau & Meuwly	Cazade & Bereau & Meuwly
density	<b>0.89</b>	<b>0.84</b>
deltaH	<b>13.51</b>	<b>12.88</b>
deltaG	<b>-6.65 +/- 0.34</b>	<b>-5.72 +/- 0.32</b>

Scaling

1  
1.025  
1.05  
1.075  
1.1

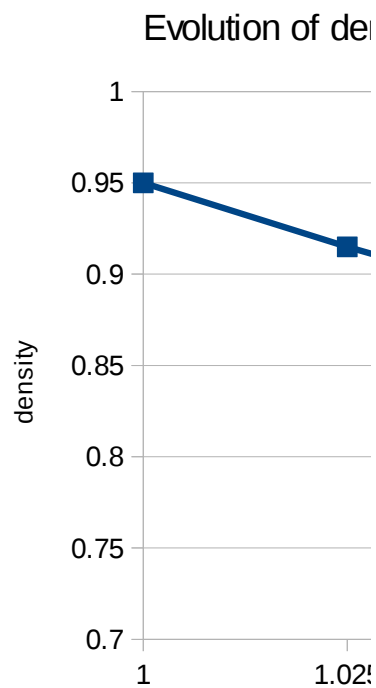
density

0.95  
0.915  
0.883  
0.843  
0.805

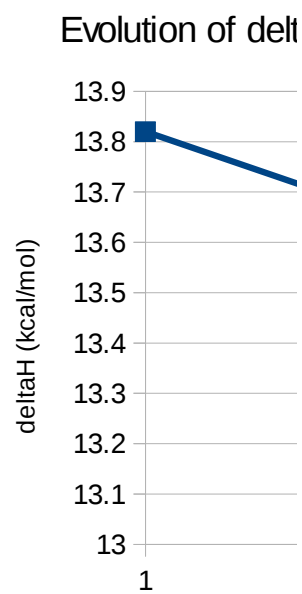
deltaH

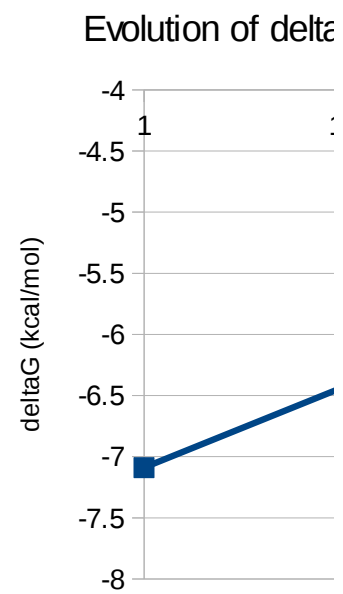
13.82  
13.68  
13.569  
13.29  
13.469



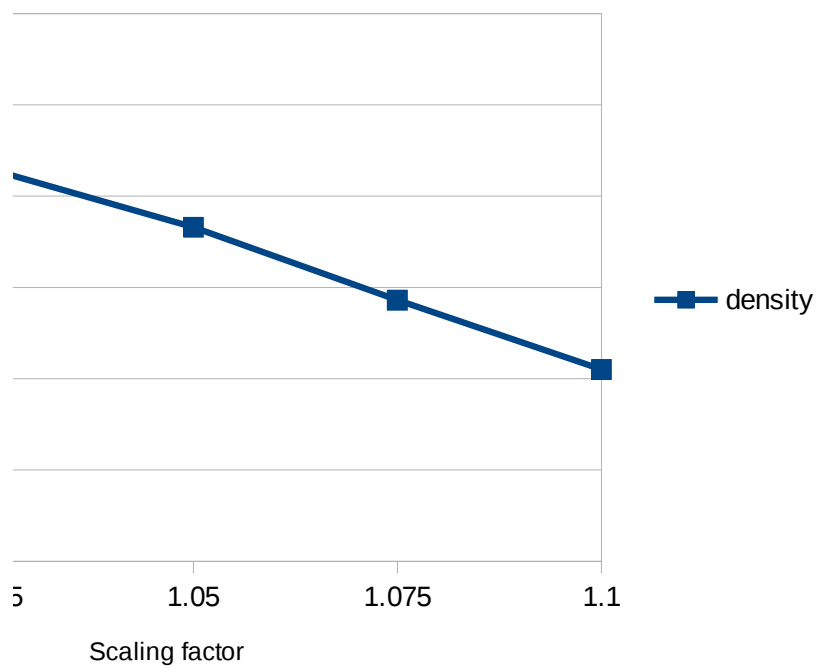


detaG
<b>-7.09</b>
<b>-6.37</b>
<b>-6.21</b>
<b>-5.68</b>
<b>-5.67</b>

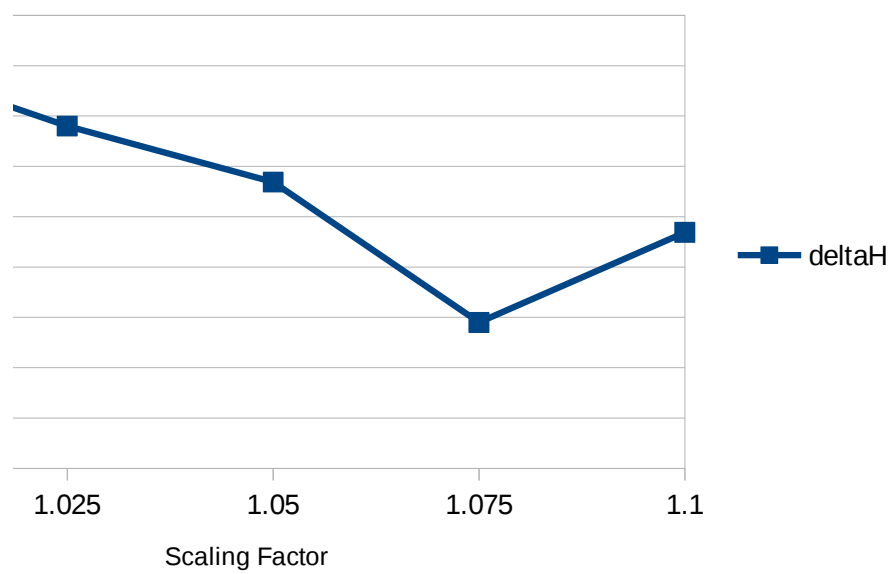




density while scaling LJ Epsilons and Sigmas



ΔH while scaling LJ parameters Epsilons and Sigmas



$\Delta G$  while scaling LJ parameters Epsilons and Sigmas

