

Thermodynamics of liquids: Standard molar entropies and heat capacities of common solvents from 2PT Molecular Dynamics

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Supplementary Materials

Appendix I. Description of forcefield potential functions

The molecules are represented explicitly (including hydrogen atoms) by interaction sites located on each nucleus. The potential energy is expressed as a sum of valence (or bonded) interactions and nonbonded interactions:

$$E_{total} = E_{valence} + E_{nonbond} \quad (\text{A.I.1})$$

The valence interactions consist of diagonal terms namely, bond stretching (E_b), bond angle bending (E_a), dihedral angle torsion (E_t), and inversion (E_v):

$$E_{valence} = E_{bond} + E_{angle} + E_{torsion} + E_{inversion} \quad (\text{A.I.2})$$

The nonbonded interactions consist of van der Waals (E_{vdw}), electrostatic (E_{Coul}) and the case of the Dreiding forcefield, hydrogen bond (E_{hb}) terms.

$$E_{nonbond} = E_{vdw} + E_{coulomb} + E_{hbond} \quad (\text{A.I.3})$$

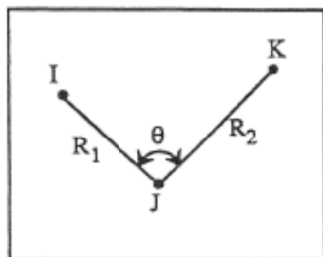
A.I.1. E_{bond}

The two-body bond stretch is a function of the bond equilibrium distance R_0 and the force constant K_b , described with a harmonic function:

$$E_b = \frac{1}{2} K_b (R - R_0)^2 \quad (\text{A.I.4})$$

A.I.2. E_{angle}

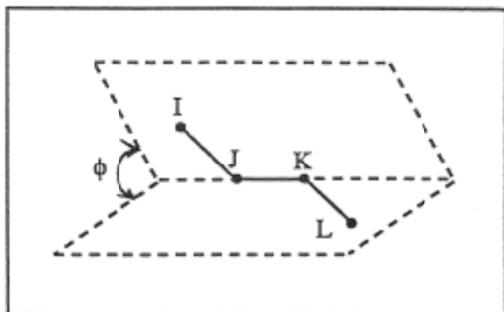
Given any two bonds to a common atom, the bond angle interaction is a function of the angle θ between them and the K_θ force constant, described with a harmonic function: Dreiding should use the cosine form



$$E_a = \frac{1}{2} K_\theta (\theta - \theta_0)^2 \quad (\text{A.I.5})$$

A.I.3. $E_{torsion}$

Given any two bonds IJ and KL attached to a common bond JK, the dihedral angle ϕ is defined as the angle between the JKL plane and the IJK plane:

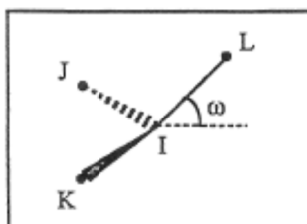


$$E_t = \sum_{n=1}^p \frac{1}{2} K_{\theta,n} [1 - d \cos(n\phi)] \quad (\text{A.I.6})$$

A positive angle is clockwise when looking from J toward K. $\phi=0^\circ$ for the cis configuration and $\phi = 180^\circ$ for the trans configuration. The torsional energy is summed over all available torsions, where each $K_{\theta,n}$ is one-half the rotational barrier, $n = 1,2,3\dots 6$ is the periodicity of the potential and $d = \pm 1$ is the phase factor ($d = +1$ when the cis conformation is the minimum while $d = -1$ when the cis conformation is maximum).

A.I.4. $E_{inversion}$

Given an atom I having exactly three distinct bonds IJ, IK, and IL (e.g. NH_3), the inversion potential is used to keep all the atoms in the same plane. For Dreiding, this potential is described using an Umbrella inversion term, where ω_0 is the angle between the IL axis and the IJK plane:

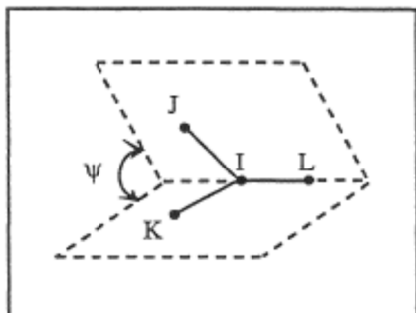


$$E_n = \frac{1}{2} C [\cos(\omega) - \cos(\omega_0)] \text{ for } \omega_0 < 0^\circ$$

where $K_\omega = C \sin^2 \omega_0$ is the force constant

$$E_n = K_\omega [1 - \cos(\omega)] \text{ otherwise} \quad (\text{A.I.7})$$

For the AMBER 2003/GAFF and OPLS AA/L forcefields, the inversion term is defined as if it were a torsion (improper torsion JILK) where K_ψ is the rotational barrier and n is the periodicity:



$$E_n = \frac{1}{2} K_\psi \cos [n(\psi - \psi_0)] \quad (\text{A.I.8})$$

A.I.5. E_{vdw}

The vdW interactions between atoms i and j are represented by the analytic Lennard-Jones 12-6 (LJ12-6) potential, with interaction energy ϵ , equilibrium distance R_0 and r being the distance between the atoms. A switching function $S(r)$ is applied that ramps the energy and force smoothly to zero between an inner (r_{inner}) and outer (r_{outer}) cutoffs:

$$E_{vdw} = \begin{cases} \varepsilon \left[\left(\frac{R_0}{r} \right)^{12} - 2 \left(\frac{R_0}{r} \right)^6 \right] & r < r_{inner} \\ \varepsilon \left[\left(\frac{R_0}{r} \right)^{12} - 2 \left(\frac{R_0}{r} \right)^6 \right] \times S_{vdw} & r_{inner} < r < r_{outer} \\ 0 & r > r_{outer} \end{cases} \quad (\text{A.I.9})$$

$$S_{vdw} = \frac{[r_{outer}^2 - r^2]^2 [r_{outer}^2 + 2r^2 - 3r_{inner}^2]}{[r_{outer}^2 - r_{inner}^2]^3}$$

vdW interactions with 1-2 and 1-3 bonded neighbors are ignored while the interactions between 1-4 bonded neighbors (atoms in a torsion) are scaled by 0.5 for the AMBER 2003/GAFF and OPLS AA/L forcefields and 1.0 for Dreiding.

A.I.6. E_{Coul}

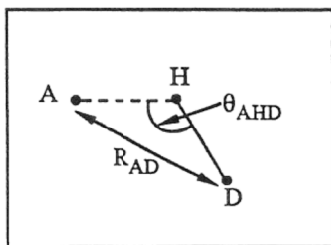
The electrostatic interactions between atoms i and j are separated into a long range contribution calculated by the PPPM¹ method and a real space contribution calculated from the Coulombic formula:

$$E_{coul} = \frac{q_i q_j}{\varepsilon_0 r} \quad (\text{A.I.10})$$

where $(1/\varepsilon_0) = 332.056$ converts units so that energy is in kcal/mol, the charge is in electron units, and r is the distance in Å between the atoms. Electrostatic interactions with 1-2 and 1-3 bonded neighbors are ignored while the interactions between 1-4 bonded neighbors are scaled by 0.833 for AMBER 2003/GAFF, 0.5 for OPLS AA/L and 1.0 (no scaling) for Dreiding.

A.I.7. E_{hb}

The Dreiding force field has an explicit term describing atoms involved in a hydrogen bond. Here, R_{AD} is the radial distance between the donor (D) and acceptor (A) atoms and θ_{AHD} the bond angle between the acceptor (A), the hydrogen (H) and the donor (D). The hydrogen bond is then described as:



$$E_{hb} = D_0 \left[5 \left(\frac{R_0}{R_{AD}} \right)^{12} - 6 \left(\frac{R_0}{R_{AD}} \right)^{10} \right] \cos^4(\theta_{AHD}) \quad (\text{A.I.11})$$

with equilibrium distance R_0 and interaction energy D_0 . We have added the Dreiding hbond potential to the open source LAMMPS² MD package.

Appendix II. Calculation of physical properties from MD

A.II.1. Bulk Density ρ

The average bulk density $\langle \rho \rangle$ (g/cm^3) is a test of the R_0 of the van der Waals parameters in the forcefield and is calculated³ from 5 1ns windows over the entire production dynamics from the window averaged volume $\langle V \rangle$ according to

$$\langle \rho \rangle = \frac{512 \times M_{\text{liquid}}}{N_a \times \langle V \rangle} = \frac{512 \times M_{\text{liquid}}}{0.6023 \times \langle V \rangle} \quad (\text{A.II.1a})$$

The fluctuation in the density is then obtained from the variance:

$$\delta \langle \rho \rangle = \langle \rho \rangle \frac{\delta \langle V \rangle}{\langle V \rangle} \quad (\text{A.II.1b})$$

A.II.2. Self-diffusion constant D

The self-diffusion constant D was obtained using two complementary approaches:

1. From the center of mass (COM) mean squared displacement r^2 (Einstein's relation⁴):

$$\langle r^2 \rangle = 6Dt \quad (\text{A.II.2a})$$

2. From the Green-Kubo VAC formulism⁴ in linear response theory:

$$D = \frac{1}{N} \sum_1^N \int_0^\infty \langle v_i(t) \cdot v_i(0) \rangle dt \quad (\text{A.II.2b})$$

where t is time, v_i is the axial COM velocity of molecule i and the brackets denote an autocorrelation that is summed over all molecules.

Self diffusion constants are calculated by 5 additional runs of 100 ps, using the NVT ensemble, with the atomic coordinates saved every 1ps.

A.II.3. Static dielectric constant ϵ_0

For isotropic systems in the canonical ensemble, the frequency dependent dielectric constant is given by^{5,6}

$$\frac{\epsilon(\omega) - \epsilon_\infty}{\epsilon_0 - \epsilon_\infty} = 1 - i\omega \int_0^\infty e^{-i\omega t} \Phi(t) dt \quad (\text{A.II.3a})$$

where

$$\Phi(t) = \frac{(\langle \vec{M}(t) \cdot \vec{M}(0) \rangle - \langle \vec{M} \rangle^2)}{\langle \Delta M \rangle^2} \quad (\text{A.II.3b})$$

is the dielectric decay function and

$$\Delta M = (\langle M \rangle^2 - \langle \bar{M} \rangle^2) \quad (\text{A.II.3c})$$

is the total dipole moment fluctuations.

The static dielectric constant is a test of the accuracy in the atomic charges used in the forcefield and defined in linear response theory to be

$$\epsilon_0 - \epsilon_\infty = \frac{4\pi\langle \Delta M^2 \rangle}{3Vk_B T} \quad (\text{A.II.4a})$$

Under Ewald boundary conditions, Neumann and Steinhauser⁶ showed that the equation A.II.4a has to be modified to

$$\epsilon_0^{correct} = \frac{(Q + 2)(\epsilon_0 - 1) + 3}{(Q - 1)(\epsilon_0 - 1) + 3} \quad (\text{A.II.4b})$$

where Q is determined from the real space Ewald cutoff r_c and the Ewald parameter η

$$Q = \int_0^{r_c} 4\pi r^2 dr \left(\frac{\eta}{\sqrt{\pi}} \right)^3 e^{-\eta^2 r^2} = erf(\eta r_c) - \frac{2}{\sqrt{\pi}} r_c e^{-\eta^2 r^2} \quad (\text{A.II.4c})$$

In our calculations, $Q = 0.9994$, leading to a negligible change in ϵ_0 . We note that effects due to charge polarization are neglected, as none of the forcefields considered here are polarizable.

A.II.4. Isothermal compressibility κ_T

Under isothermal conditions, the relative volume change in response to pressure is the compressibility. This is a test of the curvature of the van der Waals parameters. From classical statistic mechanics, it is defined to be:

$$\kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T \quad (\text{A.II.5a})$$

This quantity can be obtained during MD by the volume fluctuation formula³:

$$\kappa_T = \frac{\langle V^2 \rangle - \langle V \rangle^2}{k_B \langle T \rangle \langle V \rangle} \quad (\text{A.II.5b})$$

A.II.5. Coefficient of thermal expansion α_p

The coefficient of thermal expansion α_p is a test of the balance between the electrostatic and van der Waals nonbond parameters and is defined as

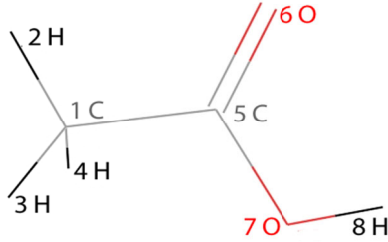
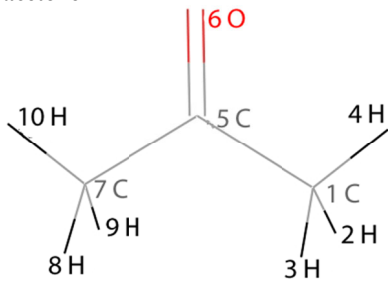
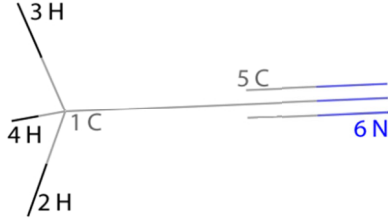
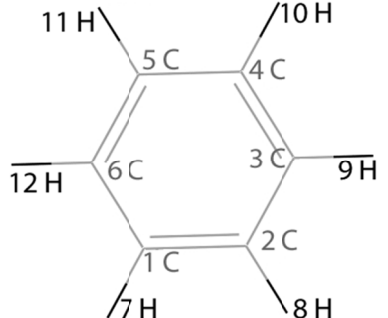
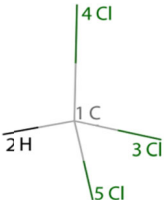
$$\alpha_p = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_p \quad (\text{A.II.6a})$$

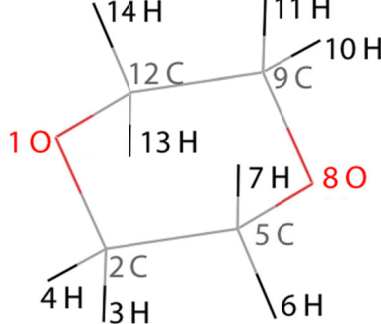
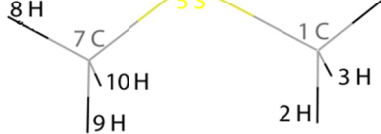
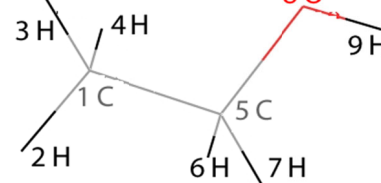
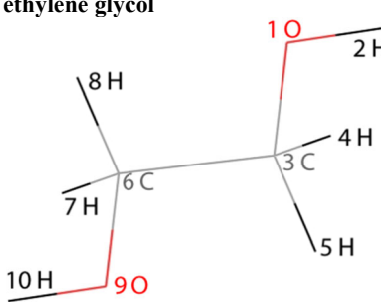
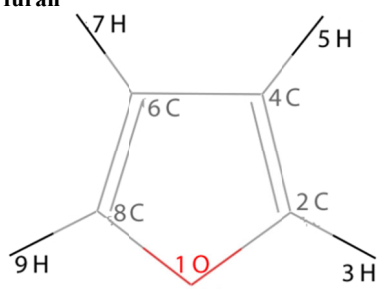
It can be calculated from MD simulations by the enthalpy-volume fluctuation formula

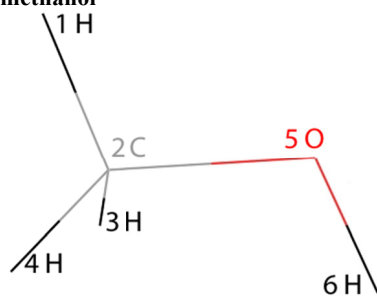
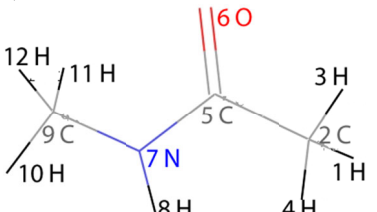
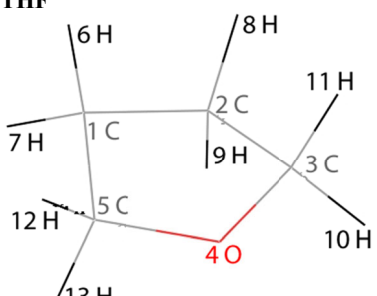
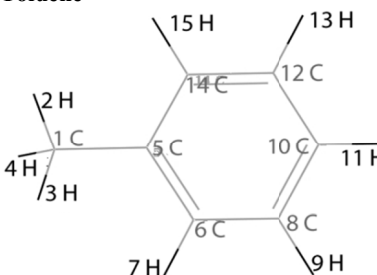
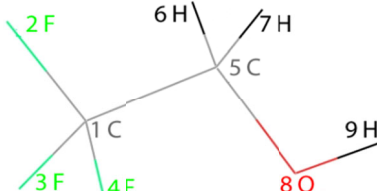
$$\alpha_p = \frac{\langle VH \rangle - \langle V \rangle \langle H \rangle}{k_B \langle T \rangle^2 \langle V \rangle} \quad (\text{A.II.6b})$$

Tables

Table S1: Forcefield Parameters (forcefield types – FFtype and atomic charges) for each liquid

Liquid	Atom #	Amber 2003/GAFF		Dreiding		OPLS AA/L ^c		
		FFtype	q(e) ^a	FFtype	q(e) ^b	FFtype	q(e)	
	1	CT/c3	-0.414320	C_3	-0.517430	CT	-0.180000	
	2–4	HC/hc	0.127940	H_	0.186320	HC	0.060000	
	5	C/c	0.869200	C_R	0.452040	C	0.520000	
	6	O/o	-0.617290	O_R	-0.402940	O	-0.440000	
	7	OH/oh	-0.668320	O_2	-0.464690	OH	-0.530000	
	8	HO/ho	0.456910	H__A	0.374060	HO	0.450000	
		1	CT/c3	-0.294100	C_3	-0.479140	CT	-0.180000
		2–4	HC/hc	0.077200	H_	0.170510	HC	0.060000
5		C/c	0.682500	C_2	0.362770	CO4	0.470000	
6		O/o	-0.557800	O_2	-0.427550	O	-0.470000	
7		CT/c3	-0.293800	C_3	-0.479140	CT	-0.180000	
8–10		HC/hc	0.077200	H_	0.170510	HC	0.060000	
		1	CT/c2	-0.236658	C_3	-0.530570	CT	-0.080000
		2–4	HC/hc	0.114711	H_	0.227860	HC	0.060000
	5	CY/c1	0.382240	C_1	0.302060	CZ	0.460000	
	6	NY/n1	-0.489715	N_1	-0.455070	NZ	-0.560000	
		1–6	CA/ca	-0.129400	C_R	-0.130430	CA	-0.115000
7–12		HA/ha	0.129400	H_	0.130430	HA	0.115000	
	1	CT/c3	-0.384700	C_3	-0.446920	CT	-0.333600	
	2	H3/h3	0.265900	H_	0.272260	HC	0.297600	
	3–5	Cl/cl	0.039600	Cl	0.058220	Cl	0.012000	

1,4 dioxane	1, 8 2, 5, 9, 12 3, 4, 6, 7, 10, 11, 13, 14	OS/os CT/c3 H1/h1	-0.424600 0.103300 0.054500	O_3 C_3 H_	-0.348680 -0.107365 0.140853	OS CT HC	-0.400000 0.140000 0.030000	
	DMSO	1, 7 2 - 4 8 - 10 5 6	CT/c3 H1/h1 S/s4 O/O	-0.262450 0.125527 0.307524 -0.517786	C_3 H_ S_3 O_2	-0.601566 0.189727 0.768190 -0.703420	CT HC SZ OZ	-0.035000 0.060000 0.170000 -0.460000
	ethanol	1 2 - 4 5 6, 7 8 9	CT/c3 HC/hc CT/c3 H1/h1 OH/oh HO/ho	-0.086100 0.024600 0.413200 -0.060600 -0.695100 0.415400	C_3 H_ C_3 H_ O_3 H__A	-0.495100 0.157400 -0.088920 0.126010 -0.499380 0.359180	CT HC CT HC OH HO	-0.180000 0.060000 0.145000 0.060000 -0.683000 0.418000
	ethylene glycol	1, 9 2, 10 3, 6 4, 5, 7, 8	OH/oh HO/ho CT/c3 H1/h1	-0.710400 0.432600 0.221000 0.028400	O_3 H__A C_3 H_	-0.507110 0.359080 -0.147670 0.147850	OH HO CT HC	-0.683000 0.418000 0.145000 0.060000
	furan	1 2, 8 3, 9 4, 6 5, 7	OS/os CA/cc H4/h4 C*/cd HA/ha	-0.176000 -0.033600 0.159100 -0.195700 0.158200	O_R C_R H_ C_R H_	-0.279120 0.072480 0.150090 -0.196380 0.113370	OA C5A HA C5BC HA	-0.190000 -0.019000 0.142000 -0.154000 0.126000
								

methanol 	1, 3, 4	H1/h1	0.037200	H_	0.144520	HC	0.040000	
	2	CT/c3	0.116600	C_3	-0.273960	CT	0.145000	
	5	OH/oh	-0.649700	O_3	-0.506980	OH	-0.683000	
	6	HO/ho	0.421500	H__A	0.347380	HO	0.418000	
NMA 	1, 3, 4	HC/hc	0.017300	H_	0.170560	HC	0.060000	
	2	CT/c3	-0.041100	C_3	-0.533770	CT	-0.180000	
	5	C/c	0.586900	C_R	0.421960	C	0.500000	
	6	O/o	-0.591100	O_2	-0.529550	O	-0.500000	
	7	N/n	-0.419200	N_R	-0.338550	N	-0.500000	
	8	H/hn	0.282300	H__A	0.317470	H	0.300000	
	9	CT/c3	-0.207800	C_3	-0.360920	CT	0.020000	
	10 - 12	H1/h1	0.112700	H_	0.170560	HC	0.060000	
	THF 	1, 2	CT/c3	-0.017180	C_3	-0.368460	CT	-0.120000
		3, 5	CT/c3	0.294740	C_3	0.019710	CT	0.140000
4		OS/os	-0.607000	O_3	-0.718900	OS	-0.400000	
6 - 9		HC/hc	0.012880	H_	0.182695	HC	0.060000	
10 - 13		H1/h1	0.000090	H_	0.171405	HC	0.030000	
Toluene 	1	CT/c2	-0.241400	C_3	-0.494260	CT	-0.065000	
	2 - 4	HC/hc	0.075700	H_	0.159540	HC	0.060000	
	5	CA/ca	0.115700	C_R	0.073590	CA	-0.115000	
	6, 14	CA/ca	-0.147800	C_R	-0.137468	CA	-0.115000	
	8, 12	CA/ca	-0.191000	C_R	-0.137468	CA	-0.115000	
	10	CA/ca	-0.092200	C_R	-0.137468	CA	-0.115000	
	7, 15	HA/ha	0.127400	H_	0.125878	HA	0.115000	
	9, 13	HA/ha	0.145300	H_	0.125878	HA	0.115000	
	11	HA/ha	0.123000	H_	0.125878	HA	0.115000	
	TFE 	1	CT/c3	0.503100	C_3	0.855690	CT	0.532300
		2 - 4	F/f	-0.179000	F_	-0.302700	F	-0.205700
5		CT/c3	0.047700	C_3	-0.164910	CT3	0.126300	
6, 7		H1/h1	0.071000	H_	0.169580	HC	0.082500	
8		OH/oh	-0.586800	O_3	-0.493350	OH	-0.635100	
9		HO/ho	0.431000	H__A	0.371710	HO	0.428600	

^a RESP⁷ Charge scheme for HF/6-31G* geometry optimization

^b Mulliken⁸ population analysis from HF/6-31G* geometry optimization

^c As determined by the Macromodel 7.0 program

Table S2: Comparison of calculated heat of vaporization ΔH_{vap} (kcal/mol) for all 15 liquids and 4 forcefields

	Exp ^a	AMBER 2003	Dreiding	GAFF	OPLS AA/L
acetic acid	12.49		5.6 ± 0.10		11.66 ± 0.01
acetone	7.39	7.37 ± 0.01	6.71 ± 0.02	7.28 ± 0.01	6.70 ± 0.01
acetonitrile	7.86	7.60 ± 0.01	7.69 ± 0.01	7.20 ± 0.01	6.37 ± 0.00
benzene	8.09	6.67 ± 0.02	7.13 ± 0.02	6.27 ± 0.04	7.13 ± 0.02
chloroform	7.46	6.02 ± 0.01	6.24 ± 0.02	6.29 ± 0.01	6.69 ± 0.02
dioxane	9.23	10.90 ± 0.01	7.98 ± 0.01	10.84 ± 0.02	8.27 ± 0.02
DMSO	11.26	12.29 ± 0.03	11.18 ± 0.12	12.11 ± 0.02	13.05 ± 0.01
ethanol	10.11	10.23 ± 0.01	11.50 ± 0.03	11.03 ± 0.02	9.87 ± 0.01
ethylene glycol	15.27	19.99 ± 0.01	26.86 ± 0.04	20.90 ± 0.02	20.72 ± 0.04
furan	6.56	6.51 ± 0.02	6.22 ± 0.01	6.66 ± 0.02	6.46 ± 0.03
methanol	8.95	9.33 ± 0.01	16.43 ± 0.07	10.04 ± 0.01	8.85 ± 0.00
NMA	13.30 ^b	14.54 ± 0.01	17.17 ± 0.08	14.30 ± 0.02	13.88 ± 0.02
THF	7.65	9.06 ± 0.02	10.10 ± 0.05	8.96 ± 0.01	5.77 ± 0.02
toluene	9.08	7.45 ± 0.01	7.83 ± 0.03	7.51 ± 0.02	8.21 ± 0.01
TFE	10.51 ^c	10.87 ± 0.04	11.10 ± 0.02	11.81 ± 0.02	12.44 ± 0.02

^a Reference⁹

^b Reference¹⁰

^c Reference¹¹

Table S3: Comparison of calculated coefficients of thermal expansion α_p ($\times 10^4$ K⁻¹) for all 15 liquids and 4 forcefields

	AMBER 2003	Dreiding	GAFF	OPLS AA/L
acetic acid		5.440 ± 0.880		7.000 ± 0.918
acetone	15.241 ± 0.837	16.743 ± 3.286	15.332 ± 1.759	12.703 ± 1.303
acetonitrile	17.813 ± 1.953	15.105 ± 1.057	17.953 ± 1.244	31.648 ± 4.758
benzene	14.729 ± 2.929	10.788 ± 4.202	19.717 ± 1.976	10.740 ± 0.537
chloroform	16.310 ± 0.966	12.099 ± 1.959	15.464 ± 0.571	16.146 ± 2.376
1,4 dioxane	10.098 ± 1.682	11.572 ± 2.771	10.917 ± 1.340	13.565 ± 1.025
DMSO	12.065 ± 0.607	10.066 ± 0.733	9.355 ± 1.443	10.751 ± 0.801
ethanol	15.372 ± 1.900	26.081 ± 4.856	17.386 ± 2.995	11.898 ± 1.911
ethylene glycol	6.332 ± 0.468	3.689 ± 1.665	4.650 ± 1.753	9.041 ± 1.754
furan	12.000 ± 1.030	11.511 ± 1.135	10.634 ± 0.998	14.011 ± 1.077
methanol	12.803 ± 1.146	16.938 ± 4.128	11.029 ± 1.139	13.629 ± 1.333
NMA	8.515 ± 1.028	11.156 ± 1.207	10.229 ± 1.154	9.069 ± 0.620
THF	13.164 ± 2.593	9.399 ± 1.003	11.277 ± 2.310	19.680 ± 1.379
toluene	13.297 ± 1.188	9.258 ± 1.009	11.928 ± 0.712	13.273 ± 0.973
TFE	15.698 ± 2.074	12.695 ± 2.731	11.602 ± 1.570	17.269 ± 1.492

Table S4: Comparison of calculated isothermal compressibilities κ_T ($\times 10^6 \text{ atm}^{-1}$) for all 15 liquids and 4 forcefields

	AMBER 2003		Dreiding		GAFF		OPLS AA/L	
acetic acid			51.20	± 5.01			55.60	± 5.34
acetone	119.00	± 5.54	186.00	± 22.40	124.00	± 11.20	130.00	± 8.71
acetonitrile	133.00	± 6.90	118.00	± 10.40	144.00	± 11.60	398.00	± 51.00
benzene	123.00	± 22.90	81.10	± 32.00	164.00	± 29.80	79.70	± 5.76
chloroform	169.00	± 7.29	132.00	± 12.50	154.00	± 4.11	139.00	± 27.30
1,4 dioxane	47.20	± 6.60	98.00	± 15.70	61.70	± 7.93	87.30	± 6.67
DMSO	58.30	± 1.87	57.60	± 5.38	52.10	± 5.97	47.20	± 3.12
ethanol	121.00	± 4.86	319.00	± 50.40	146.00	± 20.50	97.40	± 3.98
ethylene glycol	23.40	± 0.87	53.90	± 13.00	31.70	± 9.22	44.10	± 4.85
furan	106.00	± 10.10	100.00	± 9.02	81.50	± 5.00	104.00	± 12.00
methanol	105.00	± 7.20	265.00	± 38.80	91.30	± 5.08	119.00	± 10.40
NMA	52.50	± 5.17	104.00	± 13.50	55.80	± 3.76	58.40	± 2.89
TFE	145.00	± 10.60	87.90	± 14.90	93.50	± 8.24	165.00	± 14.80
THF	79.30	± 12.80	56.70	± 4.15	60.40	± 14.30	202.00	± 23.10
toluene	121.00	± 13.20	80.40	± 4.52	105.00	± 10.30	110.00	± 8.50

Table S5: ΔC_v (cal/mol/K) corrections to C_v to obtain C_p according to equation (1)

	AMBER 2003	Dreiding	GAFF	OPLS
acetic acid		0.10		0.08
acetone	0.23	0.19	0.22	0.14
acetonitrile	0.20	0.16	0.20	0.22
benzene	0.25	0.21	0.35	0.20
chloroform	0.21	0.21	0.20	0.23
dioxane	0.27	0.21	0.24	0.29
DMSO	0.27	0.19	0.18	0.27
ethanol	0.17	0.23	0.18	0.13
ethylene glycol	0.14	0.02	0.06	0.16
furan	0.13	0.16	0.15	0.21
methanol	0.09	0.08	0.08	0.10
NMA	0.16	0.16	0.22	0.16
TFE	0.20	0.21	0.17	0.20
THF	0.26	0.21	0.26	0.27
toulene	0.25	0.19	0.23	0.26

Figures

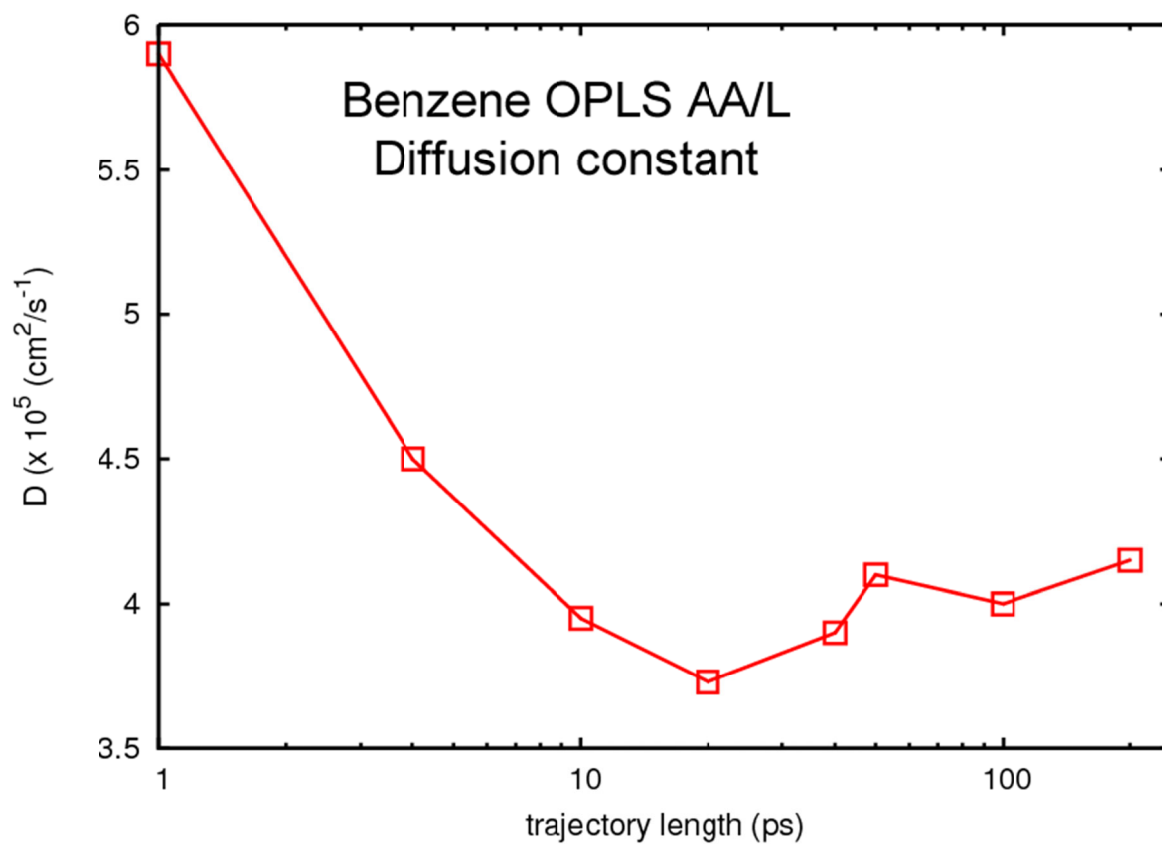


Figure S1: Convergence of the self-diffusion constant D ($\times 10^5 \text{ cm}^2/\text{s}^{-1}$) of benzene using the OPLS AA/L forcefield, calculated with the 2PT method and the Green-Kubo VACF approach. Convergence is observed after 50ps.

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