Supplementary Information

Van der Waals Interactions in Non-Polar Liquids

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Table S.1 Experimental data for pure compounds.

Compound	A_{vdw} (Å^2)	V_{vdw} (Å^3)	T_m (K)	T_c (K)	V_0 (Å^3)	V_t (Å^3)	V_c (Å^3)	E_{exp} (kJ mol^{-1})	$-\Delta G^*$ (kJ mol^{-1})	$-\Delta H^*$ (kJ mol^{-1})	$T\Delta S^*$ (kJ mol^{-1})	$\Delta G_{w>o}$ (kJ mol^{-1})	$\Delta G_{o>w}$ (kJ mol^{-1})	$\Delta G_{hex>w}$ (kJ mol^{-1})
HELIUM	18.7	7.5		5										8.6
NEON	24.6	11.3	25	44	19.8	25.9	34.6	0.9		1.6				9.1
ARGON	41.8	25.2	84	151	35.7	46.9	62.5	2.9		6.3				11.5
KRYPTON	49.7	32.8	116	209	43.8	57.4	76.6	4.1		8.5				13.3
XENON	59.2	42.7	161	290	53.9	70.9	94.4	5.6		11.9				14.2
METHANE	51.2	32.8	91	190	46.4	58.6	82.4	3.6		8.0				13.5
ETHANE	73.4	52.4	90	305	65.7	76.1	122.9	5.5						17.4
PROPANE	93.7	72.0	85	370	88.6	99.3	168.3	6.6						21.1
N-BUTANE	113.8	91.8	135	425	111.7	131.1	212.0	7.6						24.9
N-PENTANE	133.9	111.3	143	470	133.7	156.5	258.9	8.2	13.8	27.7	13.5	19.0	28.4	28.8
N-HEXANE	154.1	131.1	178	507	155.5	187.7	306.9	8.6	16.4	32.9	16.0	18.7	32.2	32.9
N-HEPTANE	174.1	150.6	182	540	177.8	213.5	358.5	9.1	19.1	38.1	18.5	18.8	36.3	36.1
N-OCTANE	194.2	170.3	216	569	200.8	247.0	408.9	9.6	21.7	43.1	20.8	18.4	39.7	40.0
N-NONANE	214.3	190.0	220	594			457.6		24.3	45.6	20.6	18.6	43.5	
N-DECANE	234.4	209.6	243	617	248.2	307.7	504.5	10.5	26.8	53.1	25.3	18.5	49.8	
N-UNDECANE	254.4	229.3	247	639			555.0		29.5	57.3	26.8	18.4	53.3	
N-DODECANE	274.6	249.0	263	658	296.1	367.9	603.1	11.2	32.0	63.0	29.7	18.4	53.7	
N-TRIDECANE	294.2	268.4	268	676			651.7		34.0	70.6	34.3	18.4		
N-TETRADECANE	313.7	287.9	279	697			699.4		37.0	78.0	38.8			
N-PENTADECANE	333.2	307.2	283	707			747.8		40.8	85.9	43.6			
N-HEXADECANE	352.9	326.8	291	721	389.8	486.4	795.9	12.2	42.4	94.9	49.4	18.1		
N-HEPTADECANE	372.4	346.1	295	733			834.2							
N-OCTADECANE	392.1	365.7	301	745			831.0							
N-NONADECANE	411.7	385.0	305	756			934.4							

N-EICOSANE	431.3	404.6	309	767			938.7						
N-HENEICOSANE	450.9	423.9	314	782			993.7						
N-DOCOSANE	470.6	443.4	317	792			1039.8						
N-TRICOSANE	490.1	462.7	321	801			1085.6						
N-TETRACOSANE	509.8	482.3	324	810			1131.3						
N-PENTACOSANE	529.4	501.6	327	819			1177.0						
N-HEXACOSANE	549.1	521.1	329	827			1222.9						
N-HEPTACOSANE	568.6	540.4	332	835			1268.4						
N-OCTACOSANE	588.4	560.0	334	843			1314.2						
N-NONACOSANE	607.9	579.4	337	850			1359.9						
N-TRIACONTANE	627.6	598.8	339	857			1405.8						
ISOBUTANE	111.7	91.6	113	408			218.1						
ISOPENTANE	129.6	111.0	113	460	134.5	152.3	253.8	8.1	13.1	24.8	11.3	19.5	28.1
NEOPENTANE	127.5	111.3	256	434	134.4	190.8	251.8	7.2		22.6	10.8		29.0
2-METHYLPENTANE	149.7	130.6	119	497			304.6		15.6	29.1	13.0	19.2	31.6
3-METHYLPENTANE	147.4	130.3	110	504	157.0	175.8	304.3	8.6	15.9	29.4	13.0	19.1	31.8
2,2-DIMETHYLBUTANE	143.1	130.3	173	489			297.9		14.6	27.1	12.0	19.4	30.9
2,3-DIMETHYLBUTANE	144.0	130.3	144	500			296.9		15.4	28.3	12.5	19.4	30.6
2-METHYLHEXANE	169.8	150.2	155	530			349.5		18.2			18.5	36.2
3-METHYLHEXANE	165.6	150.1	154	535			334.8		18.4			19.3	35.2
3-ETHYLPENTANE	162.9	149.9	154	540			346.0		18.5				
2,2-DIMETHYLPENTANE	160.2	149.8	149	520			345.9		17.0				34.8
2,3-DIMETHYLPENTANE	158.3	149.5		537			326.5		18.1				34.4
2,4-DIMETHYLPENTANE	164.8	150.1	154	520			347.4		17.2	31.9	14.2	19.1	35.0
3,3-DIMETMYLPENTANE	158.3	149.5	139	536			343.2		17.7				34.1
2,2,3-TRIMETHYLBUTANE	156.0	148.9	248	531			330.2		17.2			17.4	
2-METHYLHEPTANE	189.8	169.9	164	559			405.8		20.7				
3-METHYLHEPTANE	185.3	168.3	153	564			385.1		20.9				39.4
4-METHYLHEPTANE	185.2	168.3	152	562			396.2		20.8				
3-ETHYLHEXANE	182.7	169.5		565			378.3		20.8				
2,2-DIMETHYLHEXANE	183.2	169.5	152	550			397.5		19.5				
2,3-DIMETHYLHEXANE	181.2	169.2		563			388.9		20.4				
2,4-DIMETHYLHEXANE	182.9	169.4		553			392.5		19.8			18.3	

2,5-DIMETHYLHEXANE	185.5	169.7	182	550			399.5		19.8				
3,3-DIMETHYLHEXANE	178.0	169.1	147	562			367.5		20.0				
3,4-DIMETHYLHEXANE	179.5	168.9		569			386.8		20.7				
2-METHYL-3-ETHYLPENTANE	179.6	168.8	158	567			368.2		20.4				
3-METHYL-3-ETHYLPENTANE	173.0	168.5	182	576			378.1		20.5				
2,2,3-TRIMETHYLPENTANE	173.5	167.2	161	563			361.9		19.7				
2,2,4-TRIMETHYLPENTANE	177.8	169.3	166	544	196.2	229.9	389.0	9.4	18.6	33.9	14.7	19.7	36.6
2,3,3-TRIMETHYLPENTANE	170.7	168.0	172	573			377.6		20.2				
2,3,4-TRIMETHYLPENTANE	173.4	167.3	164	566			382.3		20.2			19.0	37.4
2,2,3,3-TETRAMETHYLBUTANE	166.1	167.1		568			382.5		20.6				
2-METHYLOCTANE	207.9	188.5	193	587			449.3		23.4			18.2	
3-METHYLOCTANE	203.5	188.4	165	590			438.6		23.4			18.3	
4-METHYLOCTANE	203.3	188.2	160	588			435.0		23.2				44.5
3-ETHYLHEPTANE	200.8	187.9		594			432.9		23.1				
2,2-DIMETHYLHEPTANE	201.9	188.5	160	577			430.9		22.0				
2,6-DIMETHYLHEPTANE	204.0	188.5	170	576			444.9		22.4			18.2	
2,2,3-TRIMETHYLHEXANE	193.1	187.4		591			418.1		22.0				
2,2,4-TRIMETHYLHEXANE	193.0	187.7	153	574			426.8		21.2				
2,2,5-TRIMETHYLHEXANE	197.8	188.1	167	568			430.7		21.0	38.9	17.3	18.7	39.6
2,3,3-TRIMETHYLHEXANE	191.2	187.2	156	599			419.6		22.3				
2,3,5-TRIMETHYLHEXANE	195.9	187.7	145	582			428.9		21.9				
2,4,4-TRIMETHYLHEXANE	191.0	187.4	160	582			427.6		21.6				
3,3,4-TRIMETHYLHEXANE	189.1	186.9	172	604			410.2		22.6				
3,3-DIETHYLPENTANE	187.2	187.0	240	610			392.0		23.2				
2,2-DIMETHYL-3-ETHYLPENTANE	190.1	187.3	174	589			424.2		22.0				
2,4-DIMETHYL-3-ETHYLPENTANE	188.3	186.9	151	591			425.0		22.3				
2,2,3,3-TETRAMETHYLPENTANE	182.4	186.4	263	611			396.1		22.5				
2,2,3,4-TETRAMETHYLPENTANE	186.3	187.1	152	592			406.6		20.7				
2,2,4,4-TETRAMETHYLPENTANE	186.6	187.5	206	571			417.6		20.6				
2,3,3,4-TETRAMETHYLPENTANE	184.0	186.7	171	607			404.9		22.6				
2-METHYLNONANE	227.7	207.9	198	609			499.4		26.0				
3-METHYLNONANE	225.6	207.6	188	614			490.6		26.0				
4-METHYLNONANE	225.5	207.6	174	619			469.9		25.7				

5-METHYLNONANE	225.6	207.7	185	610			484.0		25.6					
2,7-DIMETHYLOCTANE	223.7	207.8	219	600			493.5		25.1			18.1		
3,3,4-TRIMETHYLHEPTANE	208.5	206.3		628			459.5		24.7					
3,3,5-TRIMETHYLHEPTANE	208.8	206.6		609			467.6		24.1					
2,2,3,3-TETRAMETHYLHEXANE	202.0	205.8	219	623			472.1		24.4					
2,2,5,5-TETRAMETHYLHEXANE	211.4	207.5	260	581			474.6		22.3					
2,4-DIMETHYL-3-ISOPROPYL-PENTANE	204.3	205.5	191	614			464.0		24.2					
CYCLOPROPANE	82.0	61.9	146	398			135.2		9.2					17.5
CYCLOBUTANE	100.1	80.0	182	460			174.5		12.6					
CYCLOPENTANE	116.2	98.2	179	512	112.2	135.5	214.2	8.6	15.4	27.6	11.6	18.6	25.1	25.9
CYCLOHEXANE	131.3	117.1	280	553	134.8	181.6	256.0	9.0	17.9	34.5	16.0	20.5	28.1	28.7
CYCLOHEPTANE	146.7	136.4	265	604	155.7	200.2	297.7	9.9	21.3				30.0	
CYCLOOCTANE	160.3	155.1	288	647	176.3	227.2	338.0	10.7	24.3				33.6	
CYCLONONANE	173.9	173.5	284	682			380.2							
CIS-DECAHYDRONAPHTHALENE	180.9	181.3	230	702	205.1	243.1	399.2	12.2	28.7	53.2	23.5	17.7	39.6	
TRANS-DECAHYDRONAPHTMALENE	184.4	181.8	243	687			397.9		27.6					
METHYLCYCLOPROPANE	102.2	81.5	96	437			183.6							
ETHYLCYCLOPROPANE	122.1	101.2	124	482			235.5							
CIS-1,2-DIMETHYLCYCLOPROPANE	120.7	101.0	132	484			235.5							
TRANS-1,2-DIMETHYLCYCLOPROPANE	122.2	101.1	123	469										
METHYLCYCLOBUTANE	119.7	99.8		487			226.8							
ETHYLCYCLOBUTANE	138.2	119.3	130	527			272.5							
METHYLCYCLOPENTANE	135.0	118.0	131	533			264.3		17.0	30.5	12.9	18.3	28.8	
ETHYLCYCLOPENTANE	153.2	137.5	135	569			311.3		19.7			18.2		
1,1-DIMETHYLCYCLOPENTANE	147.2	136.4	203	547			300.8		18.1					
CIS-1,2-DIMETHYLCYCLOPENTANE	149.3	137.1	219	565			306.9		19.3					
TRANS-1,2-DIMETHYLCYCLOPENTANE	151.8	137.5	155	553			299.3		18.5					
CIS-1,3-DIMETHYLCYCLOPENTANE	153.8	137.6	139	551			300.8		18.4					
TRANS-1,3-DIMETHYLCYCLOPENTANE	153.7	137.6	139	553			300.8		18.5					
N-PROPYLCYCLOPENTANE	173.0	157.0	156	603			352.4		22.3				37.0	
ISOPROPYLCYCLOPENTANE	168.1	156.7	162	593			348.5		21.6			18.3		
1-METHYL-1-ETHYLCYCLOPENTANE	164.6	156.4	129	582			355.1		21.1					
CIS-l-METHYL-2-ETHYL-CYCLOPENTANE	165.0	155.4	167	592			355.2		21.9					

TRANS-l-METHYL-2-ETHYL-CYCLOPENTANE	169.1	156.7	167	581	355.1	21.1	
CIS-l-METHYL-3-ETHYL-CYCLOPENTANE	171.5	156.9		581	355.2	21.1	
TRANS-1-METHYL-3-ETHYL-CYCLOPENTANE	168.7	156.4		581	355.2	21.1	
1,1,2-TRIMETMYLCYCLOPENTANE	161.5	155.3	251	570	355.2	20.3	
1,1,3-TRIMETMYLCYCLOPENTANE	165.9	155.7	131	557	355.2	19.4	35.5
l,CIS-2,CIS-3-TRIMETHYL-CYCLOPENTANE	163.8	155.4	157	584	355.1	21.3	
l,CIS-2,TRANS-3-TRIMETHYL-CYCLOPENTANE	164.3	155.4	161	576	355.2	20.7	
l,TRANS-2,CIS-3-TRIMETHYL-CYCLOPENTANE	166.8	155.9	160	566	355.2	19.9	
l,CIS-2,CIS-4-TRIMETHYL-CYCLOPENTANE	167.4	155.5	141	575	355.2	20.7	
l,CIS-2,TRANS-4-TRIMETMYL-CYCLOPENTANE	165.9	155.6	140	576	355.2	20.6	
l,TRANS-2,CIS-4-TRIMETHYL-CYCLOPENTANE	168.7	155.9	142	564	355.2	19.9	
N-BUTYLCYCLOPENTANE	191.0	175.2	165	621	400.9		
ISOBUTYLCYCLOPENTANE	186.4	175.2	158	624	379.0		
1-METHYL-1-n-PROPYL-CYCLOPENTANE	183.0	174.8		606	400.9		
1,1-DIETHYLCYCLOPENTANE	178.3	174.5		612	401.0		
CIS-1,2-DIETHYLCYCLOPENTANE	183.3	174.7	155	617	400.9		
1,1-DIMETHYL-2-ETHYL-CYCLOPENTANE	177.3	174.6		594	400.9		
N-PENTYLCYCLOPENTANE	212.0	195.8	190	644	446.7		44.7
N-HEXYLCYCLOPENTANE	231.5	215.1	200	665	492.4		
N-HEPTYLCYCLOPENTANE	251.1	234.5	220	684	538.3		
N-OCTYLCYCLOPENTANE	270.7	254.0	229	701	583.9		
N-NONYLCYCLOPENTANE	290.3	273.4	244	717	629.7		
N-DECYLCYCLOPENTANE	309.9	292.8	251	732	675.5		
N-UNDECYLCYCLOPENTANE	329.5	312.3	263	746	721.1		
N-OODECYLCYCLOPENTANE	349.2	331.7	268	759	767.0		
N-TRrDECYLCYCLOPENTANE	368.8	351.1	278	771	812.6		
N-TETRADECYLCYCLOPENTANE	388.4	370.6	282	782	858.4		
N-PENTADECYLCYCLOPENTANE	408.0	389.9	290	792	904.1		
N-HEXADECYLCYCLOPENTANE	427.6	409.4	294	803	950.2		
N-HEPTADECYLCYCLOPENTANE	447.1	428.8	300	811	995.7		
N-OCTADECYLCYCLOPENTANE	466.8	448.3	303	821	1041.6		
N-NONADECYLCYCLOPENTANE	486.3	467.6	308	829	1087.2		
N-EICOSYLCYCLOPENTANE	506.0	487.1	311	836	1132.9		

METHYLCYCLOHEXANE	146.6	136.4	146	572	306.1	19.4	18.3	31.9
ETHYLCYCLOHEXANE	167.2	156.1	162	609	373.5	22.2		
1,1-DIMETHYLCYCLOHEXANE	161.5	155.7	240	591	373.6	20.8		
CIS-1,2-DIMETHYLCYCLOHEXANE	162.2	155.7	223	606	381.6	21.9		34.3
TRANS-1,2-DIMETHYLCYCLOHEXANE	164.6	156.0	183	596	382.3	21.2		
CIS-I,3-DIMETMYLCYCLOHEXANE	167.1	156.3	197	591	373.6	20.9		
TRANS-1,3-DIMETHYLCYCLOHEXANE	164.4	156.0	183	598	382.2	21.4		
CIS-I,4-DIMETHYLCYCLOHEXANE	164.5	156.0	186	598	382.2	21.4		
TRANS-1,4-DIMETHYLCYCLOHEXANE	167.2	156.4	236	590	372.9	20.8		35.4
N-PROPYLCYCLOHEXANE	186.8	175.6	178	639	396.1	24.7		
ISOPROPYLCYCLOHEXANE	181.3	175.4	184	636	390.3	24.4		
N-BUTYLCYCLOHEXANE	206.2	194.9	198	667	476.6	27.2		
ISOBUTYLCYCLOHEXANE	200.6	194.3		660	439.3	26.1		
SEC-BUTYLCYCLOHEXANE	198.4	194.7		650	431.3			
TERT-BUTYLCYCLOHEXANE	193.3	193.9	232	645	423.7			
1-METHYL-4-ISOPROPYL-CYCLOHEXANE	198.1	194.2		637	431.3			
N-PENTYLCYCLOHEXANE	225.8	214.3	216	670	483.6			
N-HEXYLCYCLOHEXANE	245.3	233.7	230	688	529.3			
N-HEPTYLCYCLOHEXANE	264.9	253.1	243	706	575.3			
N-OCTYLCYCLOHEXANE	284.6	272.6	253	723	620.8			
N-NONYLCYCLOHEXANE	304.2	291.9	263	738	666.7			
N-DECYLCYCLOHEXAME	323.8	311.4	271	751	712.4			
N-UNDECYLCYCLOHEXANE	343.4	330.8	279	764	758.1			
N-DODECYLCYCLOHEXANE	363.0	350.2	286	776	804.0			
N-TRIDECYLCYCLOHEXANE	382.6	369.6	292	787	849.5			
N-TETRADECYLCYCLOHEXANE	402.1	389.0	297	797	895.2			
N-PENTADECYLCYCLOHEXANE	421.6	408.4	302	807	941.4			
N-HEXADECYLCYCLOHEXANE	441.3	427.9	307	817	986.8			
N-MEPTADECYLCYCLOHEXANE	460.8	447.3	311	825	1032.8			
N-OCTADECYLCYCLOHEXANE	480.5	466.8	314	833	1078.6			
N-NONADECYLCYCLOHEXANE	500.0	486.2	318	841	1124.0			
N-EICOSYLCYCLOHEXANE	520.0	506.0	322	849	1170.8			
ETHYLCYCLOHEPTANE	181.8	175.1		640	383.3			

BICYCLOHEXYL	218.4	220.3	277	727	496.0	33.1				
1-METHYL-[CIS-DECAHYDRO-NAPHTHALENE]	194.8	199.4		755	448.4					
1-METHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	198.8	200.0		743	448.4					
1-ETHYL-[CIS-DECAHYDRO-NAPHTHALENE]	210.0	218.5		729	494.3					
1-ETHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	214.0	219.2		714	494.2					
9-ETHYL-[CIS-DECAHYDRONAPHTHALENE]	206.8	217.9		721	494.2					
9-ETHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	207.3	218.0		709	494.2					
PERFLUOROMETHANE	72.4	50.0	90	228	116.3					
PERFLUOROETHANE	102.4	78.3	173	293	186.0					
PERFLUOROPROPANE	128.9	106.2	90	345	248.6					
N-PERFLUOROBUTANE	154.7	133.9	145	386	314.2					
ISO-PERFLUOROBUTANE	150.3	133.2		395						
N-PERFLUOROPENTANE	180.6	161.6	148	421	382.9					40.7
N-PERFLUOROHEXANE	206.1	189.3	187	448	465.1	20.1	34.3	19.3	20.2	47.3
N-PERFLUOROHEPTANE	232.2	217.0	235	487	546.2	22.7	35.4	18.6	19.0	52.7
N-PERFLUOROOCTANE	257.9	244.5	213	499	595.5	24.6				58.0
N-PERFLUORONONANE	283.8	272.2	208	524	656.9	26.8				59.0
N-PERFLUORODECANE	309.6	299.9	309	542	705.9					
N-PERFLUOROUNDECANE	335.4	327.6	330							
N-PERFLUORODODECANE	361.1	355.2	348							
N-PERFLUOROICOSANE	567.5	576.3	433							
PERFLUOROCYCLOBUTANE	137.5	114.7	235	388	269.9					
PERFLUOROCYCLOPENTANE	158.0	140.6	284	424	350.5	17.6				
PERFLUOROCYCLOHEXANE	176.6	167.4	324	457	367.1	20.4				
PERFLUOROMETHYLCYCLOHEXANE	198.5	194.6	228	486	431.0	21.9	37.7	20.4		
CIS-PERFLUORODECALIN	239.0	254.9	262	565		28.1	47.0	28.8		

[1] A_{vdW} and V_{vdW} were calculated for a single extended conformation of each molecule using B3LYP and a 6-31G* basis set in Spartan 08 (Wavefunction Inc).
[2] T_m, T_c and V_c were obtained from *Technical data book - petroleum refining*, 4th ed., American Petroleum Institute, Washington D. C., 1983, and *Dechema DTherm database*, accessed via the United Kingdom Chemical Database Service.
[3] The polynomial coefficients for liquid density and the Antoine coefficients for vapour density from [2] were used to determine V_0, V_t and E_{exp}.
[4] ΔG^*_{298}, ΔH^* and $T\Delta S^*_{298}$ are from A. Ben-Naim, in *Solvation Thermodynamics*, Plenum Press, 1987, and A. Ben-Naim, Y. Marcus, *J. Chem. Phys*., 1984, **81**, 2016.
[5] $\Delta G_{w>o}$, $\Delta G_{o>w}$ and $\Delta G_{hex>w}$ were calculated from solubility data from M. H. Abraham, *J. Am. Chem. Soc*. 1982, **104**, 2085, and Y. Marcus, in *The Properties of Solvents*, Wiley, Chichester, 1998.

Table S.2 Experimental transfer free energies for mixtures of cyclohexane and *cis*-decalin at 298 K.

		$\Delta G_{o>o'}$ (kJ mol^{-1})	
$\chi_{cyclohexane}$	$\chi_{cis\text{-}decalin}$	cyclohexane	*cis*-decalin
0.000	1.000		0.0
0.371	0.629	0.0	-0.4
0.453	0.547	0.0	0.0
0.481	0.519	0.0	0.0
0.561	0.439	0.0	0.6
0.585	0.415	0.0	-0.1
0.603	0.397	0.0	0.5
0.693	0.307	0.0	-0.3
0.740	0.260	0.0	-0.2
0.811	0.189	0.0	0.0
0.906	0.094	0.0	0.1
0.953	0.047	0.0	-1.5
0.995	0.005	0.0	-1.7
1.000	0.000	0.0	

T. Boublik, G. C. Benson, *Can. J. Chem.* 1972, **50**, 1978.

Table S.3 Experimental transfer free energies for mixtures of cyclohexane and *n*-hexane at 303 K.

		$\Delta G_{o>o'}$ (kJ mol^{-1})	
$\chi_{cyclohexane}$	$\chi_{n\text{-}hexane}$	cyclohexane	*n*-hexane
0.000	1.000		0.0
0.098	0.902	-0.2	0.0
0.201	0.799	-0.2	0.0
0.233	0.768	-0.2	0.0
0.352	0.648	-0.1	0.0
0.518	0.482	-0.1	-0.1
0.603	0.397	-0.1	-0.1
0.652	0.348	0.0	-0.1
0.709	0.291	0.0	-0.1
0.801	0.199	0.0	-0.2
0.907	0.093	0.0	-0.2
1.000	0.000	0.0	

M. Goral, P. Oracz, S. Warycha, *Fluid Phase Equil.* 1998, **152**, 109.

Table S.4 Experimental transfer free energies for mixtures of cyclohexane and *n*-heptane at 313 K.

		$\Delta G_{o>o'}$ (kJ mol^{-1})	
$\chi_{cyclohexane}$	$\chi_{n\text{-heptane}}$	cyclohexane	*n*-heptane
0.000	1.000		0.0
0.054	0.946	-0.1	0.0
0.101	0.899	-0.1	0.0
0.147	0.854	-0.1	0.0
0.199	0.802	-0.1	0.0
0.248	0.752	-0.1	0.0
0.298	0.702	-0.1	0.0
0.348	0.652	0.0	0.0
0.398	0.602	0.0	0.0
0.449	0.551	0.0	0.0
0.450	0.550	0.0	0.0
0.498	0.502	0.0	0.0
0.501	0.500	0.0	0.0
0.544	0.456	0.0	-0.1
0.550	0.450	0.0	0.0
0.599	0.401	0.0	-0.1
0.600	0.400	0.0	-0.1
0.650	0.350	0.0	-0.1
0.700	0.300	0.0	-0.1
0.750	0.250	0.0	-0.1
0.799	0.201	0.0	-0.1
0.850	0.150	0.0	-0.1
0.902	0.099	0.0	-0.2
0.953	0.047	0.0	-0.2
1.000	0.000	0.0	

J. J. Segovia, M. C. Martin, C. R. Chamorro, M. A. Villamanan, *J. Chem. Eng. Data* 1998, **43**, 1021.

Table S.5 Experimental transfer free energies for mixtures of *n*-hexane and *n*-hexadecane at 298 K.

		$\Delta G_{o>o'}$ (kJ mol^{-1})	
$\chi_{n\text{-hexane}}$	$\chi_{n\text{-hexadecane}}$	*n*-hexane	*n*-hexadecane
1.000	0.000	0.0	
0.708	0.292	0.0	
0.648	0.352	0.1	
0.626	0.374	0.0	
0.738	0.262	0.0	
0.430	0.570	0.1	
0.663	0.337	0.1	
0.635	0.365	0.0	
0.478	0.522	0.1	
0.222	0.778	0.0	
0.000	1.000	0.0	

J. H. Hildebrand, J. W. Sweny, *J. Phys. Chem.* 1939, **43**, 297.

Table S.6 Experimental transfer free energies for mixtures of *n*-perfluorohexane and *n*-hexane at 298 K.

		$\Delta G_{o>o'}$ (kJ mol^{-1})	
$\chi_{n\text{-perfluorohexane}}$	$\chi_{n\text{-hexane}}$	*n*-perfluorohexane	*n*-hexane
0.000	1.000		0.0
0.051	0.949	5.9	0.1
0.099	0.901	5.0	0.1
0.183	0.817	3.6	0.4
0.280	0.720	2.6	0.7
0.373	0.627	1.9	1.0
0.389	0.611	1.8	1.1
0.546	0.454	1.0	1.8
0.714	0.286	0.4	2.8
0.791	0.210	0.2	3.4
0.859	0.141	0.1	3.9
0.950	0.050	0.0	4.7
1.000	0.000	0.0	

R. D. Dunlap, R. D. Bedford, J. C. Woodbrey, S. D. Furrow, *J. Am. Chem. Soc*. 1959, **81**, 2927.

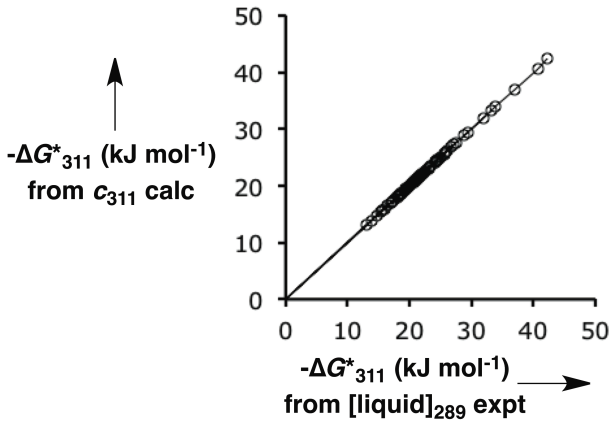

Fig. S1 Comparison of values of ΔG^* at 311 K obtained using experimental concentrations of the liquids at 289 K and using the value of c_T calculated using Equations 2, 6 and 11 at 311 K as the concentration of the liquid. The line corresponds to $y = x$.

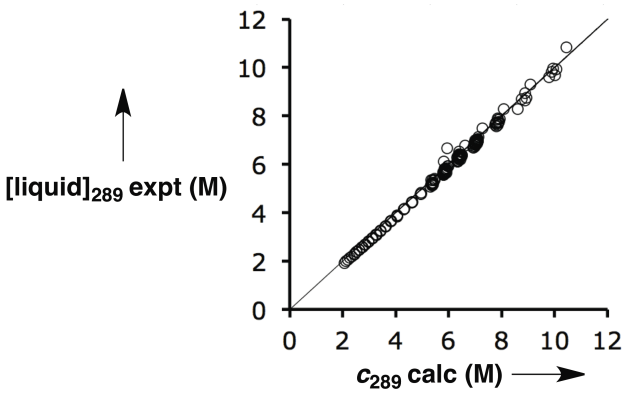

Fig. S2 Comparison of the experimental concentrations of liquids at 289 K and the values of c_T calculated using Equations 2, 6 and 11 at 289 K. The line corresponds to $y = x$.