

Supporting Information

Hypothetical Thermodynamic Properties: Vapor pressures and Vaporization Enthalpies of the Even n-Alkanes from C₄₀ to C₇₆ at T = 298.15 K by Correlation–Gas Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?

James Chickos, Tracy Wang* and Esseim Sharma**

All enthalpies reported in kJ•mol⁻¹

Table S1A. Retention Times

T/K	555.7	560.8	565.8	570.6	575.8	580.6	585.6
Run 1	t/min						
CH ₂ Cl ₂	0.781	0.81	0.516	0.795	0.798	0.794	0.815
tetracosane	1.018	1.017	0.704	0.955	0.938	0.914	0.928
octacosane	1.379	1.328	0.969	1.174	1.132	1.078	1.068
dotriacontane	2.261	2.068	1.584	1.676	1.567	1.443	1.369
tetratriacontane	3.679	3.228	2.531	2.443	2.23	2.001	1.81
hexatriacontane	4.38	3.805	2.998	2.809	2.536	2.245	2.014
heptatriacontane	5.256	4.519	3.572	3.262	2.912	2.547	2.261
octatriacontane	6.359	5.403	4.278	3.824	3.395	2.944	2.567
tetracontane	9.389	7.824	6.197	5.333	4.66	3.958	3.368
tetratetracontane	21.061	16.989	13.335	10.877	9.261	7.581	6.186

Table S1A. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 1	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(571 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (lit)	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (calcd)
tetracosane	-8387.8±305	16.529	69.733	121.9	122.21
octacosane	-9544.6±177	17.683	79.350	141.9	142.03
dotriacontane	-10740±159	18.93	89.288	162.5	162.52
pentatriacontane	-11535±195	19.693	95.897	178.1	176.15
hexatriacontane	-11921±185	20.168	99.107	182.9	182.76
heptatriacontane	-12277±179	20.59	102.066	187.6	188.86
octatriacontane	-12523±199	20.816	104.111	192.7	193.08
tetracontane	-13136±206	21.484	109.208		203.58±3.9
tetratetracontane	-14337±226	22.79	119.192		224.17±4.2

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJ mol}^{-1} = (2.061 \pm 0.034)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(571 \text{ K}) - (21538 \pm 1066) \quad r^2 = 0.9986 \quad 1$$

Table S1B. Retention Times

T/K	554.8	560.0	565.2	570.0	575.0	579.9	584.8
Run 2	t/min						
CH ₂ Cl ₂	0.754	0.797	0.792	0.759	0.804	0.831	0.828
tetracosane	0.994	1.004	0.982	0.924	0.949	0.964	0.943
octacosane	1.36	1.311	1.251	1.148	1.14	1.137	1.086

dotriacontane	2.248	2.044	1.876	1.659	1.568	1.511	1.394
pentatriacontane	3.679	3.195	2.842	2.433	2.214	2.059	1.846
hexatriacontane	4.386	3.771	3.304	2.809	2.518	2.316	2.051
heptatriacontane	5.27	4.486	3.877	3.27	2.893	2.629	2.302
octatriacontane	6.388	5.371	4.596	3.836	3.36	3.014	2.617
tetracontane	9.477	7.792	6.533	5.361	4.596	4.03	3.435
tetratetracontane	21.39	16.943	13.767	10.963	9.073	7.646	6.313

Table S1B. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(570 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$
Run 2				(lit)	(calcd)
tetracosane	-7821.4±230	15.524	65.024	121.9	122.03
octacosane	-9101.6±225	16.906	75.667	141.9	142.05
dotriacontane	-10405±213	18.352	86.503	162.5	162.43
pentatriacontane	-11342±188	19.372	94.293	178.1	177.08
hexatriacontane	-11707±171	19.812	97.327	182.9	182.79
heptatriacontane	-12052±159	20.215	100.196	187.6	188.18
octatriacontane	-12363±151	20.556	102.781	192.7	193.04
tetracontane	-13024±138	21.311	108.276		203.38±1.85
tetratetracontane	-14298±128	22.75	118.868		223.30±2.02

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJ mol}^{-1} = (1.8808 \pm 0.016)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(570 \text{ K}) - (0.268 \pm 0.558) \quad r^2 = 0.9996 \quad 2$$

Table S2A. Retention Times

T/K	556.7	561.7	566.6	571.7	576.6	581.5	586.5
Run 3	t/min						
CH ₂ Cl ₂	0.627	0.624	0.621	0.627	0.629	0.629	0.616
pentatriacontane	2.878	2.461	2.132	1.883	1.674	1.507	1.361
hexatriacontane	3.43	2.899	2.483	2.167	1.904	1.695	1.516
heptatriacontane	4.117	3.44	2.915	2.514	2.185	1.923	1.704
octatriacontane	4.965	4.106	3.443	2.937	2.524	2.197	1.929
tetracontane	7.31	5.931	4.882	4.08	3.434	2.928	2.523
dotetracontane	10.89	8.689	7.034	5.771	4.773	3.993	3.379
tetratetracontane	16.308	12.834	10.225	8.258	6.719	5.527	4.603
hexatriacontane	24.526	19.04	14.987	11.934	9.565	7.755	6.361
octatriacontane	36.89	28.304	21.999	17.299	13.69	10.953	8.862
pentacontane	55.343	42.071	32.353	25.148	19.659	15.525	12.414

Table S2A. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(572 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$
Run 3				(lit)	(calcd)
pentatriacontane	-12134±96	20.995	100.877	178.1	177.62
hexatriacontane	-12458±98	21.359	103.571	182.9	182.79
heptatriacontane	-12785±101	21.728	106.290	187.6	188.00
octatriacontane	-13109±103	22.091	108.983	192.7	193.17
tetracontane	-13750±103	22.812	114.312	203.5	203.39

dotetracontane	-14384±102	23.522	119.583		213.49±2.54
tetratetracontane	-15013±103	24.228	124.812	223.7	223.52
hexatriacontane	-15624±100	24.904	129.892		233.26±2.73
octatriacontane	-16230±100	25.575	134.930		242.92±2.83
pentacontane	-16822±92	26.227	139.852		252.36±2.93

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJmol}^{-1} = (1.918\pm 0.021)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(572 \text{ K}) - (15.831\pm 0.41) \quad r^2 = 0.9995 \quad (3)$$

Table S2B. Retention Times

<i>T</i> /K	555.2	560.2	565.1	570.2	575.2	580.1	585
Run 4				t/min			
CH ₂ Cl ₂	0.628	0.627	0.633	0.637	0.642	0.643	0.627
dotriacontane	1.789	1.607	1.455	1.332	1.234	1.148	1.059
triacontane	2.08	1.848	1.651	1.493	1.368	1.259	1.151
tetratriacontane	2.443	2.141	1.89	1.688	1.529	1.392	1.262
pentatriacontane	2.891	2.505	2.184	1.928	1.726	1.554	1.395
hexatriacontane	3.444	2.949	2.544	2.22	1.963	1.749	1.556
heptatriacontane	4.139	3.511	2.99	2.58	2.256	1.987	1.75
octatriacontane	4.99	4.189	3.532	3.015	2.607	2.272	1.983
tetracontane	7.343	6.052	5.004	4.19	3.545	3.03	2.598
dotetracontane	10.976	8.905	7.241	5.948	4.951	4.149	3.488
tetratetracontane	16.411	13.102	10.507	8.499	6.946	5.729	4.754
hexatetracontane	24.845	19.573	15.479	12.336	9.987	8.092	6.588
octatetracontane	37.444	29.127	22.735	17.9	14.313	11.44	9.185
pentacontane	56.102	43.156	33.302	25.933	20.437	16.152	12.852

Table S2B. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 4	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(570 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (lit)	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (calcd)
dotriacontane	-10775±39	19.261	89.579	162.5	162.10
triacontane	-11114±44	19.647	92.397	167.6	167.51
tetratriacontane	-11441±40	20.013	95.116	172.7	172.72
pentatriacontane	-11768±40	20.381	97.835	178.1	177.94
hexatriacontane	-12079±35	20.724	100.420	182.9	182.90
heptatriacontane	-12416±41	21.11	103.222	187.6	188.26
octatriacontane	-12729±39	21.455	105.824	192.7	193.26
tetracontane	-13359±41	22.161	111.061	203.5	203.30
dotetracontane	-13996±40	22.876	116.357		213.46±1.72
tetratetracontane	-14614±38	23.568	121.495	223.7	223.32
hexatetracontane	-15239±50	24.265	126.691		233.28±1.86
octatetracontane	-15853±56	24.953	131.796		243.07±1.93
pentacontane	-16453±50	25.623	136.784		252.64±2.00

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJmol}^{-1} = (1.918\pm 0.014)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(570 \text{ K}) + (9.70\pm 0.40) \quad r^2 = 0.9996 \quad (4)$$

Table S3A. Retention Times

<i>T</i> /K	599.7	604.7	609.6	614.6	619.5	624.5	629.5
Run 5	t/min						
hexane	0.899	0.804	0.847	0.855	0.86	0.858	0.851
heptatriacontane	1.827	1.598	1.509	1.431	1.372	1.298	1.235
octatriacontane	2.015	1.748	1.631	1.532	1.458	1.371	1.294
tetracontane	2.481	2.106	1.932	1.791	1.674	1.547	1.453
dotetracontane	3.138	2.617	2.356	2.145	1.969	1.799	1.656
tetratetracontane	4.057	3.332	2.943	2.629	2.368	2.131	1.928
hexatetracontane	5.371	4.323	3.748	3.287	2.907	2.578	2.282
octatetracontane	7.21	5.717	4.857	4.184	3.633	3.171	2.765
pentacontane	9.752	7.631	6.373	5.396	4.613	3.971	3.383
dopentacontane	13.268	10.277	8.449	7.044	5.94	5.029	4.222
tetrapentacontane	18.165	13.963	11.281	9.273	7.714	6.436	5.349
hexapentacontane	24.863	19.032	15.141	12.262	10.091	8.332	6.847
octapentacontane	34.12	25.953	20.373	16.314	13.282	10.829	8.817

Table S3A. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 5	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(614 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (lit)	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (calcd)
heptatriacontane	-11097±223	18.594	92.256	187.6	187.69
octatriacontane	-11584±228	19.222	96.305	192.7	194.92
tetracontane	-12127±257	19.789	100.819	203.5	203.00
dotetracontane	-12745±248	20.475	105.957	213.5	212.20
tetratetracontane	-13405±242	21.231	111.444	223.3	222.03
hexatetracontane	-14138±266	22.108	117.538	233.0	232.94
octatetracontane	-14835±277	22.927	123.332	242.7	243.32
pentacontane	-15531±278	23.75	129.119	252.0	253.68
dopentacontane	-16160±268	24.463	134.348		263.05±5.5
tetrapentacontane	-16780±263	25.163	139.502		272.28±5.7
hexapentacontane	-17337±258	25.762	144.133		280.57±5.9
octapentacontane	-17908±254	26.386	148.880		289.07±6.1

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJ mol}^{-1} = (1.7908 \pm 0.040)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(614 \text{ K}) + (22.455 \pm 1375) \quad r^2 = 0.9971 \quad (5)$$

Table S3B (Run 2). Retention Times

<i>T</i> /K	607.5	612.5	617.6	622.6	627.8	632.8	637.8
Run 6	t/min						
octane	0.771	0.777	0.771	0.789	0.8	0.801	0.804
hexatriacontane	1.316	1.247	1.177	1.135	1.109	1.068	1.04
octatricontane	1.533	1.429	1.329	1.263	1.217	1.161	1.119
tetracontane	1.835	1.678	1.537	1.437	1.363	1.283	1.223
dotetracontane	2.26	2.025	1.822	1.672	1.56	1.448	1.362
tetratetracontane	2.832	2.493	2.207	1.989	1.822	1.666	1.544
hexatetracontane	3.631	3.139	2.731	2.417	2.173	1.956	1.784
octatetracontane	4.73	4.021	3.443	2.992	2.643	2.341	2.101
pentacontane	6.256	5.231	4.41	3.767	3.271	2.852	2.519

dopentacontane	8.31	6.858	5.706	4.8	4.1	3.523	3.065
tetrapentacontane	11.138	9.079	7.455	6.186	5.207	4.411	3.782
hexapentacontane	14.992	12.08	9.81	8.033	6.674	5.581	4.72
octapentacontane	20.253	16.145	12.968	10.495	8.613	7.117	5.943
hexacontane	27.449	21.663	17.211	13.783	11.186	9.142	7.542

Table S3B. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 6	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(623 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (lit)	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (calcd)
hexatriacontane	-10684±153	18.203	88.823	182.9	182.72
octatriacontane	-11302±129	18.884	93.960	192.7	193.16
tetracontane	-11902±112	19.539	98.949	203.5	203.29
dotetracontane	-12530±111	20.237	104.170	213.5	213.89
tetratetracontane	-13085±94	20.825	108.784	223.7	223.26
hexatetracontane	-13669±92	21.458	113.639	233.3	233.12
octatetracontane	-14243±90	22.078	118.411	243.0	242.81
pentacontane	-14840±94	22.735	123.374	252.5	252.89
dopentacontane	-15377±89	23.302	127.838		261.95±1.50
tetrapentacontane	-15930±88	23.893	132.436		271.29±1.54
hexapentacontane	-16466±88	24.46	136.892		280.34±1.59
octapentacontane	-17014±90	25.047	141.448		289.59±1.64
hexacontane	-17566±93	25.642	146.037		298.91±1.70

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJ mol}^{-1} = (2.031 \pm 0.012)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(623 \text{ K}) + (2.352 \pm 0.38) \quad r^2 = 0.9998 \quad (6)$$

Table S3C. Retention Times

Run 7	637.8	632.7	627.7	627.7	622.6	617.6	612.6	607.6
	t/min							
octane	0.635	0.624	0.617	0.631	0.628	0.617	0.61	0.615
dotetracontane	1.072	1.133	1.218	1.23	1.342	1.457	1.595	1.794
tetratetracontane	1.216	1.305	1.426	1.437	1.589	1.756	1.97	2.253
hexatetracontane	1.407	1.535	1.704	1.716	1.931	2.173	2.486	2.896
octatetracontane	1.657	1.839	2.075	2.089	2.388	2.738	3.191	3.775
pentacontane	1.988	2.244	2.572	2.588	3.021	3.549		
dopentacontane	2.419	2.774	3.228	3.246	3.825	4.532	5.442	6.608
tetrapentacontane	2.985	3.476	4.104	4.11	4.924	5.917	7.198	8.85
hexapentacontane	3.728	4.401	5.267	5.284	6.397	7.785	9.583	11.916
octapentacontane	4.697	5.619	6.808	6.839	8.354	10.276	12.8	16.085
hexacontane	5.966	7.222	8.835	8.876	11.052	13.867	17.736	21.972

Table S3C. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 7	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(623 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (lit)	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (calcd)
dotetracontane	-12740±64	20.807	105.915	213.5	213.958
tetratetracontane	-13305±55	21.411	110.613	223.7	223.242
hexatetracontane	-13910±69	22.077	115.642	233.3	233.182

octatetracontane	-14493±75	22.711	120.489	243.0	242.761
pentacontane	-15106±151	23.391	125.585	252.5	252.833
dopentacontane	-15571±75	23.845	129.451		260.473±3.75
tetrapentacontane	-16117±83	24.427	133.990		269.444±3.88
hexapentacontane	-16650±82	24.987	138.422		278.201±4.01
octapentacontane	-17166±84	25.524	142.711		286.679±4.13
hexacontane	-18029±148	26.609	149.886		300.858±4.34

$$\Delta_l^g H_m(298.15 \text{ K})/\text{kJ mol}^{-1} = (1.976 \pm 0.029) \Delta_{\text{sln}}^g H_m(623 \text{ K}) + (4.638 \pm 0.45) \quad r^2 = 0.9994 \quad (7)$$

Table S4A. Retention Times

<i>T/K</i>	668.3	663.2	658.2	653.1	648	642.9	637.8
Run 8	t/min						
dotetracontane	0.242	0.277	0.312	0.361	0.415	0.48	0.566
tetratetracontane	0.308	0.354	0.403	0.469	0.542	0.632	0.75
hexatetracontane	0.391	0.452	0.52	0.608	0.709	0.832	0.994
octatetracontane	0.497	0.578	0.669	0.788	0.924	1.093	1.316
pentacontane	0.631	0.738	0.861	1.02	1.206	1.435	1.739
dopentacontane	0.8	0.942	1.105	1.318	1.568	1.879	2.292
tetrapentacontane	1.013	1.2	1.418	1.7	2.038	2.458	3.019
hexapentacontane	1.283	1.527	1.817	2.192	2.644	3.212	3.97
octapentacontane	1.622	1.941	2.326	2.822	3.425	4.188	5.211
hexacontane	2.048	2.467	2.975	3.63	4.436	5.458	6.829
dohexacontane	2.582	3.127	3.794	4.657	5.726	7.092	8.926
tetrahexacontane	3.253	3.962	4.835	5.97	7.388	9.206	11.671
hexahexacontane	4.093	5.01	6.154	7.642	9.512	11.928	15.247
octahexacontane	5.146	6.333	7.823	9.77	12.238	15.427	19.762
heptacontane	6.455	7.989	9.93	12.468	15.713	19.933	25.667
doheptacontane	8.101	10.075	12.588	15.888	20.145	25.727	33.323
tetraheptacontane	10.155	12.678	15.938	20.244	25.809	33.114	43.091
hexaheptacontane	12.687	15.958	20.166	25.742	33.052	42.629	55.658

Table S4A. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 8	slope	intercept	$\Delta_{\text{sln}}^g H_m(653 \text{ K})$	$\Delta_l^g H_m(298.15 \text{ K})$ (lit)	$\Delta_l^g H_m(298.15 \text{ K})$ (calcd)
dotetracontane	-11790±142	19.069	98.017	213.5	213.35
tetratetracontane	-12378±132	19.708	102.906	223.7	223.33
hexatetracontane	-12965±129	20.347	107.786	233.3	233.30
octatetracontane	-13532±128	20.955	112.500	243.0	242.93
pentacontane	-14106±126	21.577	117.272	252.5	252.68
dopentacontane	-14651±125	22.155	121.803	261.8	261.94
tetrapentacontane	-15197±124	22.736	126.342	270.9	271.21
hexapentacontane	-15734±124	23.304	130.806	279.6	280.33

octapentacontane	-16260±124	23.857	135.179	288.3	289.27
hexacontane	-16782±117	24.403	139.519	299.9	298.13
dohexacontane	-17288±118	24.93	143.726		306.73±2.8
tetrahexacontane	-17804±123	25.472	148.015		315.49±2.9
hexahexacontane	-18324±133	26.02	152.339		324.33±3.0
octahexacontane	-18769±113	26.457	156.038		331.88±3.0
heptacontane	-19259±109	26.963	160.112		340.21±3.1
doheptacontane	-19736±116	27.451	164.077		348.31±3.2
tetraheptacontane	-20187±109	27.899	167.827		355.97±3.2
hexaheptacontane	-20656±91	28.377	171.726		363.93±3.3

$$\Delta_l^g H_m(298.15 \text{ K})/\text{kJ mol}^{-1} = (2.043 \pm 0.019) \Delta_{\text{sln}}^g H_m(653 \text{ K}) + (13.096 \pm 0.78) \quad r^2 = 0.9993 \quad (8)$$

Table S4A. Retention Times

<i>T</i> /K	637.8	643	648	653.2	658.3	663.3	668.4
Run 9	t/min						
octane	0.813	0.808	0.809	0.82	0.83	0.825	0.834
dotetracontane	1.352	1.269	1.208	1.167	1.132	1.089	1.071
tetratetracontane	1.529	1.417	1.331	1.271	1.221	1.164	1.136
hexatetracontane	1.763	1.611	1.493	1.406	1.334	1.261	1.217
octatetracontane	2.071	1.864	1.703	1.58	1.48	1.383	1.32
pentacontane	2.479	2.197	1.976	1.805	1.667	1.539	1.451
dopentacontane	3.011	2.628	2.328	2.094	1.905	1.737	1.616
tetrapentacontane	3.709	3.192	2.785	2.466	2.211	1.989	1.824
hexapentacontane	4.623	3.924	3.376	2.944	2.6	2.308	2.087
octapentacontane	5.815	4.873	4.135	3.556	3.096	2.713	2.418
hexacontane	7.378	6.11	5.119	4.342	3.729	3.225	2.836
dohexacontane	9.398	7.697	6.375	5.34	4.528	3.869	3.357
tetrahexacontane	12.028	9.75	7.992	6.615	5.544	4.684	4.012
hexahexacontane	15.432	12.403	10.059	8.244	6.832	5.71	4.833
octahexacontane	19.861	15.816	12.709	10.313	8.463	7	5.861
heptacontane	25.565	20.202	16.106	12.945	10.522	8.617	7.143
doheptacontane	32.951	25.839	20.433	16.276	13.121	10.655	8.747
tetraheptacontane	42.497	33.049	25.915	20.508	16.392	13.206	10.742
hexaheptacontane	54.706	42.276	32.937	25.874	20.483	16.4	13.205

Table S4B. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 9	slope	intercept	$\Delta_{\text{sln}}^g H_m(653 \text{ K})$	$\Delta_l^g H_m(298.15 \text{ K})$ (lit)	$\Delta_l^g H_m(298.15 \text{ K})$ (calcd)
dotetracontane	-11539±156	18.722	95.931	213.5	213.374
tetratetracontane	-12125±147	19.355	100.802	223.7	223.238
hexatetracontane	-12716±128	19.999	105.716	233.3	233.186
octatetracontane	-13296±119	20.627	110.538	243.0	242.949

pentacontane	-13881±109	21.262	115.401	252.5	252.796
dopentacontane	-14431±103	21.848	119.974	261.8	262.054
tetrapentacontane	-14979±97	22.43	124.530	270.9	271.278
hexapentacontane	-15519±92	23.002	129.019	279.6	280.368
octapentacontane	-16040±90	23.548	133.350	288.3	289.137
hexacontane	-16571±89	24.107	137.765	299.9	2980.75
dohexacontane	-17082±88	24.64	142.013		306.677±2.8
tetrahexacontane	-17586±86	25.163	146.203		315.160±2.9
hexahexacontane	-18080±84	25.672	150.310		323.476±3.0
octahexacontane	-18576±86	26.186	154.434		331.825±3.0
heptacontane	-19066±80	26.691	158.507		340.073±3.1
doheptacontane	-19547±82	27.184	162.506		348.169±3.2
tetraheptacontane	-20027±87	27.679	166.497		356.249±3.3
hexaheptacontane	-20511±76	28.179	170.520		364.396±3.3

$$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJ mol}^{-1} = (2.025 \pm 0.019)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(653 \text{ K}) + (19.143 \pm 0.8) \quad r^2 = 0.9993 \quad (9)$$

Table S14. Retention Times

<i>T</i> /K	504.65	509.55	514.65	519.65	524.75	529.75	534.75
Run 10				t/min			
CH ₂ Cl ₂	0.764	0.763	0.73	0.759	0.637	0.772	0.776
heneicosane	1.248	1.178	1.093	1.062	0.903	1.003	0.977
docosane	1.421	1.322	1.214	1.162	0.988	1.075	1.037
tricosane	1.654	1.514	1.374	1.292	1.099	1.167	1.115
tetracosane	1.967	1.769	1.584	1.463	1.244	1.287	1.215
pentacosane	2.387	2.109	1.863	1.688	1.432	1.442	1.344
hexacosane	2.949	2.561	2.231	1.983	1.678	1.643	1.51
octacosane	4.705	3.957	3.365	2.875	2.409	2.239	1.996
nonacosane	6.045	5.008	4.188	3.533	2.937	2.667	2.343
hentriacontane	10.199	8.236	6.728	5.512	4.509	3.933	3.356
dotriacontane	13.351	10.657	8.638	6.969	5.665	4.848	4.082
triacontane	17.507	13.838	11.249	8.866	7.219	6.042	5.017
tetracontane	23.029	18.036	14.626	11.333	9.209	7.565	6.203
pentatriacontane	30.342	23.501	18.828	14.499	11.669	9.469	7.689
hexatriacontane	40.047	30.7	24.254	18.605	14.809	11.899	9.576
heptatriacontane	52.576	40.12	31.82	23.946	19.145	15.093	12.027
octatriacontane	69.318	52.393	41.032	30.774	24.376	19.04	15.056

Table 14. Enthalpies of Transfer and Vaporization Enthalpies (Enthalpies in kJ mol⁻¹)

Run 10	slope	intercept	$\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(520 \text{ K})$	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (lit)	$\Delta_{\text{l}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})$ (calcd)
heneicosane	-7904.8±104	16.389	65.717	106.8	106.208
docosane	-8273.8±99	16.816	68.785	111.9	111.389
tricosane	-8641.7±96	17.243	71.844	117.0	116.553

tetracosane	-9012.8±91	17.679	74.929	121.9	121.763
pentacosane	-9390.4±86	18.128	78.068	126.8	127.064
hexacosane	-9756.1±86	18.556	81.108	131.7	132.198
octacosane	-10488±89	19.417	87.193	141.9	142.472
nonacosane	-10862±82	19.868	90.302	147.1	147.723
hentriacontane	-11597±82	20.744	96.413	157.3	158.041
dotriacontane	-11958±85	21.171	99.414	162.5	163.109
triacontane	-12280±111	21.52	102.091	167.6	167.629
tetracontane	-12621±132	21.909	104.926	172.7	172.416
pentatriacontane	-12993±120	22.364	108.019	178.0	177.638
hexatriacontane	-13370±105	22.83	111.153	182.8	182.931
heptatriacontane	-13651±141	23.107	113.489	187.5	186.876
octatriacontane	-14019±126	23.557	116.548	192.7	192.042

$$\Delta_{\text{f}}^{\text{g}}H_{\text{m}}(298.15 \text{ K})/\text{kJ mol}^{-1} = (1.689 \pm 0.008)\Delta_{\text{sln}}^{\text{g}}H_{\text{m}}(520 \text{ K}) - (4.81 \pm 0.52) \quad r^2 = 0.9997 \quad (21)$$
