

Supplement: Tables of Original Data

Table 10. Thermodynamics of Transfer of Alkylbenzenes from n-Hexadecane to the Gas Phase^a

Solute	ΔG° (kcal/mol) ^b	ΔH° (kcal/mol) ^c	$T\Delta S^\circ$ (kcal/mol) ^d
Benzene	3.81	7.27 ± 0.09 (7.26) ^e	3.46
Toluene	4.56	8.54 ± 0.10 (8.58) ^e	3.98
Ethylbenzene	5.17	9.48 ± 0.09 (9.59) ^e	4.31
n-Propylbenzene	5.78	10.44 ± 0.09 (10.55) ^e	4.66
n-Butylbenzene	6.43	11.49 ± 0.14 (11.72) ^{e,f}	5.06
n-Pentylbenzene	6.84	12.53 ± 0.33 (12.80) ^{e,f}	5.69
Change (n-Pentylbenzene to Benzene)	3.03	5.26 (5.54)	2.23

a. All data are at 25 °C. Note ΔG° and ΔS° are based on the unit molar concentration standard state.

b. Taken from Ref. 83.

c. Standard deviation obtained from ten replicate experiments.

d. Computed as $T\Delta S^\circ = \Delta H^\circ - \Delta G^\circ$.

e. Numbers in parentheses are from calorimetry (86)

f. Calculated by fitting first four data points to the linear regression equation $\Delta H^\circ = 7.363 + 1.088 * (\text{Carbon Number})$

Table 11. Thermodynamics of Transfer of Alkylbenzenes from Methanol/Water Mobile Phase to the Gas Phase^a

% MeOH		ΔG° (kcal/mol) ^b					ΔH° (kcal/mol) ^c					$T\Delta S^\circ$ (kcal/mol) ^d				
(v/v)		BZ	TL	EB	PB	BB	BZ	TL	EB	PB	BB	BZ	TL	EB	PB	BB
40		1.71	1.86	1.93	1.94	1.98	4.85	5.28	5.66	5.99	6.36	3.14	3.42	3.73	4.05	4.38
45		1.90	2.10	2.22	2.28	2.41	4.89	5.37	5.79	6.16	6.56	2.99	3.27	3.57	3.88	4.15
50		2.04	2.27	2.43	2.53	2.68	5.01	5.52	5.97	6.37	6.80	2.97	3.25	3.54	3.84	4.12
55		2.27	2.53	2.71	2.85	3.02	5.16	5.70	6.18	6.60	7.06	2.89	3.17	3.47	3.75	4.04
60		2.48	2.74	2.95	3.19	3.35	5.62	6.23	6.78	7.26	7.78	3.14	3.49	3.83	4.07	4.43
65		2.67	2.96	3.34	3.46	3.67	5.85	6.55	7.17	7.70	8.30	3.18	3.59	3.83	4.24	4.63
70		2.84	3.16	3.53	3.73	3.98	6.12	6.84	7.49	8.04	8.66	3.28	3.68	3.96	4.31	4.68
75		3.01	3.36	3.77	3.99	4.29	6.39	7.19	7.90	8.52	9.20	3.38	3.83	4.13	4.53	4.91
80		3.20	3.58	3.94	4.28	4.65	6.64	7.54	8.33	9.03	9.79	3.44	3.96	4.39	4.75	5.14
85		3.37	3.81	4.19	4.52	4.95	6.88	7.85	8.71	9.46	10.28	3.51	4.04	4.52	4.94	5.33
90		3.53	4.00	4.40	4.81	5.23	7.21	8.16	9.00	9.72	10.53	3.68	4.16	4.60	4.91	5.30
95		3.69	4.15	4.64	5.06	5.47	7.49	8.57	9.52	10.34	11.26	3.80	4.42	4.88	5.28	5.79
100		3.87	4.39	4.86	5.31	5.78	7.85	8.80	9.64	10.38	11.18	3.98	4.41	4.78	5.07	5.40

a. All data are at 25 °C in kcal/mol. b. Calculated from data in Refs. 81 - 83.

c. As measured herein. d. Computed as $T\Delta S^\circ = \Delta H^\circ - \Delta G^\circ$.

Table 12. Thermodynamics of Transfer of Alkylbenzenes from Acetonitrile/Water Mobile Phase to Gas Phase^a

% ACN (v/v)	ΔG° (kcal/mol) ^b					ΔH° (kcal/mol) ^c					$T\Delta S^\circ$ (kcal/mol) ^d				
	BZ	TL	EB	PB	BB	BZ	TL	EB	PB	BB	BZ	TL	EB	PB	BB
40	2.43	2.72	2.92	3.08	3.31	6.53	7.45	8.25	8.94	9.76	4.10	4.73	5.33	5.86	6.45
45	2.63	2.92	3.16	3.35	3.63	6.84	7.80	8.64	9.35	10.21	4.21	4.88	5.48	6.00	6.58
50	2.84	3.14	3.41	3.63	3.95	7.07	8.13	9.06	9.85	10.80	4.23	4.99	5.65	6.22	6.85
55	3.00	3.33	3.62	3.86	4.21	7.13	8.23	9.20	10.02	11.01	4.13	4.90	5.58	6.16	6.80
60	3.17	3.54	3.86	4.09	4.46	7.23	8.31	9.26	10.07	11.04	4.06	4.77	5.40	5.98	6.58
65	3.32	3.71	4.03	4.27	4.67	7.21	8.33	9.32	10.16	11.17	3.89	4.62	5.29	5.89	6.50
70	3.43	3.79	4.13	4.44	4.81	7.31	8.28	9.14	9.87	10.74	3.88	4.49	5.01	5.43	5.93
75	3.60	3.97	4.39	4.71	5.11	7.31	8.26	9.10	9.81	10.67	3.71	4.29	4.71	5.10	5.56
80	3.71	4.14	4.52	4.87	5.26	7.19	8.16	9.01	9.73	10.60	3.48	4.02	4.49	4.86	5.34
85	3.87	4.32	4.71	5.07	5.50	7.28	8.17	8.95	9.61	10.41	3.41	3.85	4.24	4.54	4.91
90	3.94	4.39	4.80	5.17	5.62	7.47	8.40	9.22	9.91	10.75	3.53	4.01	4.42	4.74	5.13
95	4.09	4.57	4.99	5.39	5.84	7.41	8.29	9.06	9.72	10.51	3.32	3.72	4.07	4.33	4.67
100	4.25	4.76	5.21	5.63	6.13	7.63	8.53	9.31	9.98	10.79	3.38	3.77	4.10	4.35	4.66

a. All data are at 25 °C in kcal/mol.

b. Calculated from data in Refs. 81-83.

c. As measured herein.

d. Computed as $T\Delta S^\circ = \Delta H^\circ - \Delta G^\circ$.