

Thermodynamic Equilibrium of Xylene Isomerization in Liquid Phase

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ASSOCIATED CONTENT

Supporting Information

Table S1. Molar thermodynamic functions, enthalpy (H) and entropy (S) at saturation pressure (P^s) for $T = (250 \text{ to } 550) \text{ K}^d$

T/K	p -Xylene ^a			m -Xylene ^b			o -Xylene ^c		
	P^s/kPa	$\Delta_0^T H/RT$	$\Delta_0^T S/R$	P^s/kPa	$\Delta_0^T H/RT$	$\Delta_0^T S/R$	P^s/kPa	$\Delta_0^T H/RT$	$\Delta_0^T S/R$
250	0.03907	17.448	26.038	0.03593	15.450	26.616	0.02716	16.129	25.690
260	0.08961	17.553	26.829	0.08300	15.635	27.419	0.06361	16.319	26.517
280	0.3836	17.783	28.368	0.3597	16.001	28.958	0.2827	16.694	28.114
298.15	1.179	18.012	29.721	1.116	16.335	30.307	0.8945	17.031	29.511
300	1.310	18.037	29.857	1.241	16.369	30.442	0.9967	17.066	29.651
320	3.739	18.311	31.304	3.572	16.743	31.884	2.922	17.440	31.138
340	9.225	18.603	32.715	8.878	17.122	33.290	7.379	17.818	32.585
360	20.22	18.913	34.098	19.58	17.510	34.667	16.50	18.201	33.997
380	40.21	19.239	35.454	39.14	17.905	36.020	33.39	18.589	35.380
400	73.78	19.578	36.789	72.15	18.308	37.351	62.20	18.984	36.738
420	126.6	19.932	38.107	124.3	18.719	38.665	108.1	19.384	38.074
440	205.3	20.299	39.409	202.2	19.14	39.96	177.3	19.79	39.39
460	317.5	20.678	40.699	313.6	19.56	41.25	276.8	20.21	40.70
480	471.6	21.069	41.979	467.1	20.00	42.52	414.7	20.63	41.99
500	677.0	21.472	43.249	672.0	20.44	43.79	599.5	21.06	43.27
520	943.9	21.885	44.512	938.8	20.89	45.06	840.8	21.50	44.54
540	1284	22.310	45.771	1279	21.36	46.33	1149	21.95	45.82
550	1485	22.528	46.401	1480	21.61	46.96	1332	22.18	46.45

^a From Chirico et al.¹. ^b From Chirico et al.². ^c From Chirico et al.³. ^d Values are presented with one digit more than justified.

Table S2. Properties and parameters for xylenes. Molecular weight (M), critical temperature (T_c), critical pressure (P_c), critical density (ρ_c), acentric factor (ω), and enthalpy of formation ($\Delta_f H^0$)

	<i>p</i> -Xylene ^a	<i>m</i> -Xylene ^b	<i>o</i> -Xylene ^c
A^d	-7.59306	-7.564368	-7.457432
B^d	1.77964	1.623819	1.519744
C^d	-1.24526	-1.139601	-1.030912
D^d	-3.93248	-4.004004	-3.997287
$M/\text{kg}\cdot\text{kmol}^{-1}$	106.167	106.167	106.167
T_c/K	616.2	617.0	630.3
P_c/kPa	3510	3540	3730
$\rho_c/\text{kg}\cdot\text{m}^{-3}$	281	283	287
ω	0.3211	0.3261	0.3107
$\Delta_f H^0/\text{kJ}\cdot\text{kmol}^{-1e}$	-24.39 ± 0.63	-25.38 ± 0.37	-24.39 ± 0.40

^a From Chirico et al.¹. ^b From Chirico et al.². ^c From Chirico et al.³. ^d Constant for eq 1. ^e Enthalpies of Formation in Liquid Phase at 298.15 K from Chirico and Steele⁴.

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