

Toluene, ethylbenzene, and cumene

Physical, transport and thermodynamic property data are presented for these important alkyl aromatics.

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Important derivatives of toluene include benzene, benzoic acid, nitrotoluenes, toluene sulfonic acids and sundry additional chemical intermediates. Major quantities of toluene are used in gasoline and as a solvent in chemical processing [4]. Ethylbenzene is primarily consumed in the production of styrene monomer for plastics, resins and coatings. Cumene is important for the production of phenol and acetone and as a blending component in fuels.

Critical properties—Table 14—1 (T/14—1)

Critical constants for toluene (methylbenzene), ethylbenzene and cumene (isopropylbenzene) are readily available [14, 415, 417, 516]. Variations of experimental results from average selected values in the table are 0.7%, 1.9% and 1.4% or less for critical temperature, pressure and volume.

Heat of vaporization—Fig. 14—1 (F/14—1)

Heat-of-vaporization data in the region of the boiling point were extended with Watson's correlation (Eq.

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See Part 1 of this series, *Chem. Eng.*, June 10, 1974, for equations starting with a boldfaced numeral "1", Part 2 for those with "2", etc. Part 2 appeared July 3; Part 3, Aug. 19; Part 4, Sept. 30; Part 5, Oct. 28; Part 6, Nov. 25; Part 7, Dec. 23, 1974; Part 8, Jan. 20, 1975; Part 9, Feb. 17; Part 10, Mar. 31; Part 11, May 12; Part 12, July 21; and Part 13, Sept. 1.

1—1) to fully cover the liquid phase for each alkyl aromatic.

Vapor pressure—F/14—2

Comprehensive vapor-pressure data from various sources were extrapolated to the melting point by means of the Cox-Antoine correlation (Eq. 1—2) to provide complete coverage of the liquid phase for the three alkyl aromatics.

Heat Capacity—F/14—3, F/14—4

Heat-capacity results are available for the ideal gas at atmospheric pressure. Agreement among the investigators is excellent, with deviations of only 1.4% for toluene and of less than 1% for ethylbenzene and toluene.

Liquid-heat-capacity data are available for only toluene and ethylbenzene. The Johnson-Huang method [14,543] was selected for estimating liquid heat capacity of cumene at 20°C. Application of the modified method to toluene and ethylbenzene produced favorable results, with deviations from experimental data of only 1%. The estimated and experimental values were extrapolated with the density relation (Eq. 1—3, $n = 1$) to fully cover the liquid phase. Average variations between

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How To Use the Graphs

Each graph is outfitted with a key that lists references and explains just what part of the curve is determined experimentally, and what part is estimated from theoretical correlations.

The shaded squares denote the following:

- Data in this region are experimentally known.
- Experimental and correlated data used.
- All data in this region are correlated.

The "regions" referred to are the temperature ranges between the melting, boiling and critical points (m.p., b.p. and c.p., respectively), or in some cases, the specific temperatures noted in the key.

Physical properties of the alkyl aromatics

Identification	Toluene	Ethylbenzene	Cumene
	$C_6H_5CH_3$	$C_6H_5C_2H_5$	$C_6H_5CH(CH_3)_2$
State (std. conditions)	Liquid	Liquid	Liquid
Molecular weight, M	92.1	106.2	120.2
Boiling point, T_b , °C	110.6	136.2	152.4
Melting point, T_m , °C	-95.0	-95.0	-96.0
Critical temp., T_c , °C	318.8	344	360
Critical pressure, P_c , atm	41.1	36.3	31.5
Critical volume, V_c , cm ³ /g-mol	316	374	434
Critical compressibility factor, Z_c	0.267	0.268	0.263

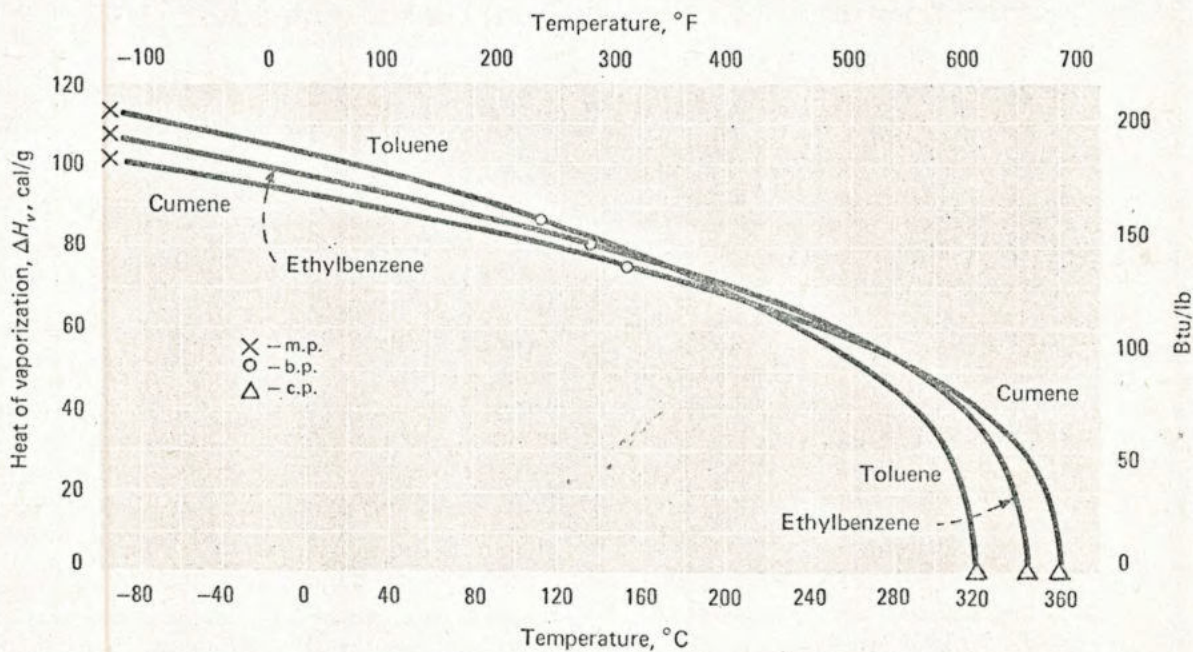
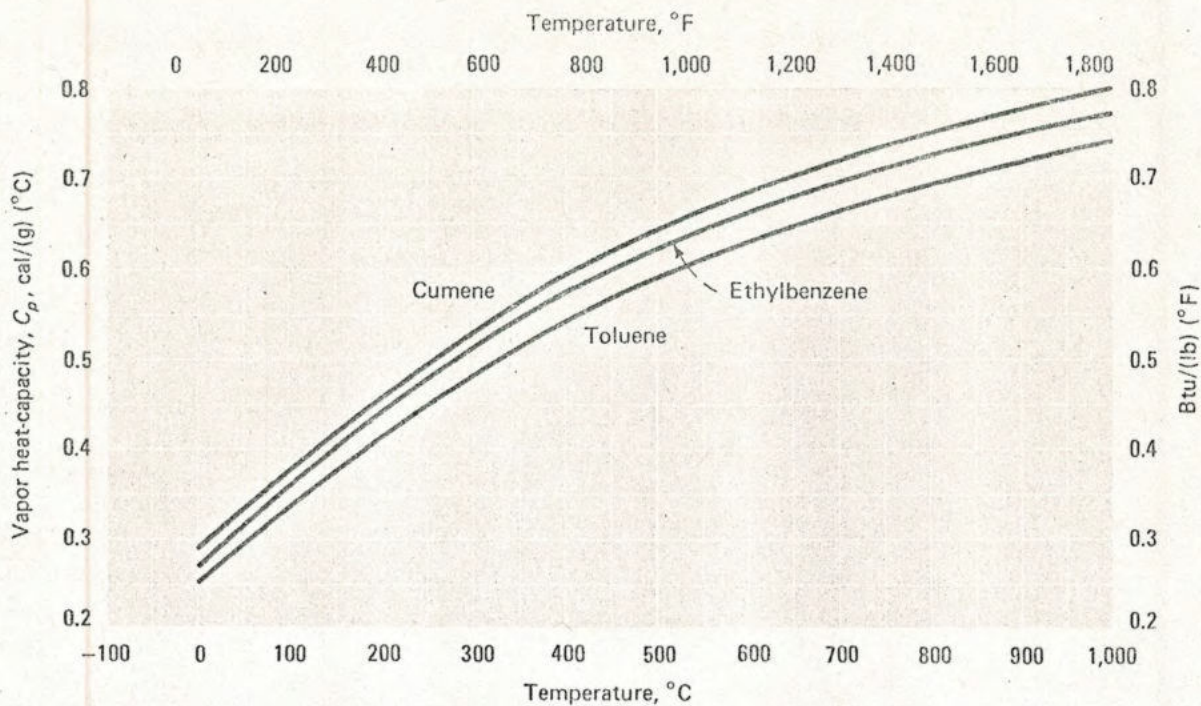


Fig. 14-1	Temperature range, C		References
	m.p. - b.p.	b.p. - c.p.	
	Toluene	<input checked="" type="checkbox"/>	
Ethylbenzene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	413, 415, 417, 419, 516
Cumene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	4, 413, 415, 417, 419, 516

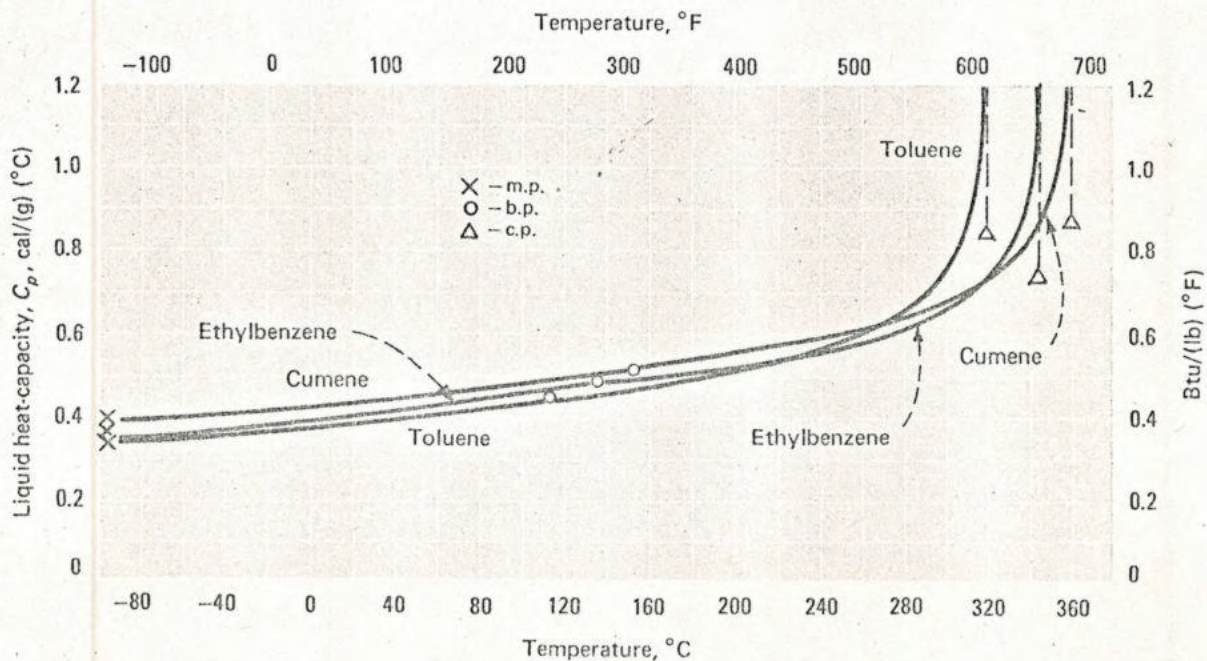
Fig. 14-2	Temperature range, C		References
	m.p. - b.p.	b.p. - c.p.	
	Toluene	<input checked="" type="checkbox"/>	
Ethylbenzene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	3, 413, 415, 417, 419, 473, 516, 529
Cumene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	3, 4, 413, 415, 417, 419, 473, 516, 529

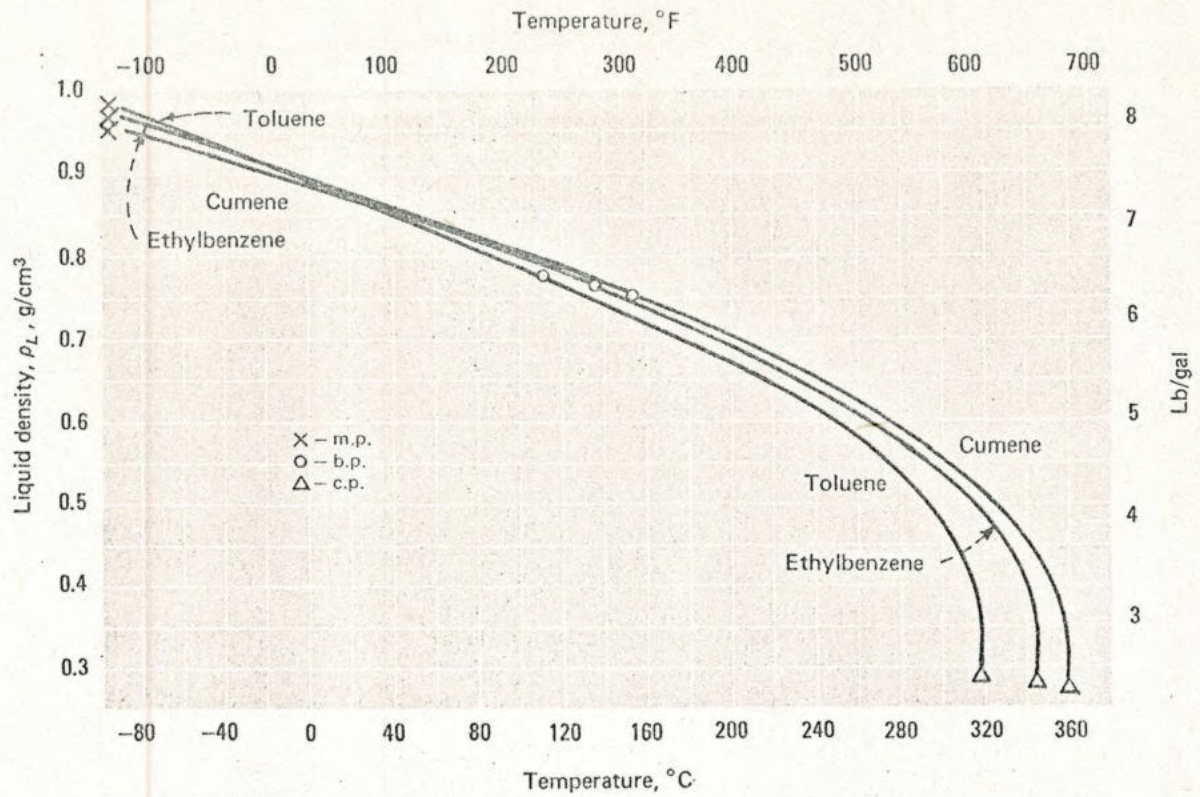




Vapor heat capacity			
Fig. 14-3	Temperature range, C		References
	0-500	500-1,000	
Toluene	☑	☑	3,15,19,417,516
Ethylbenzene	☑	☑	3,15,417,516
Cumene	☑	☑	3,15,417,516

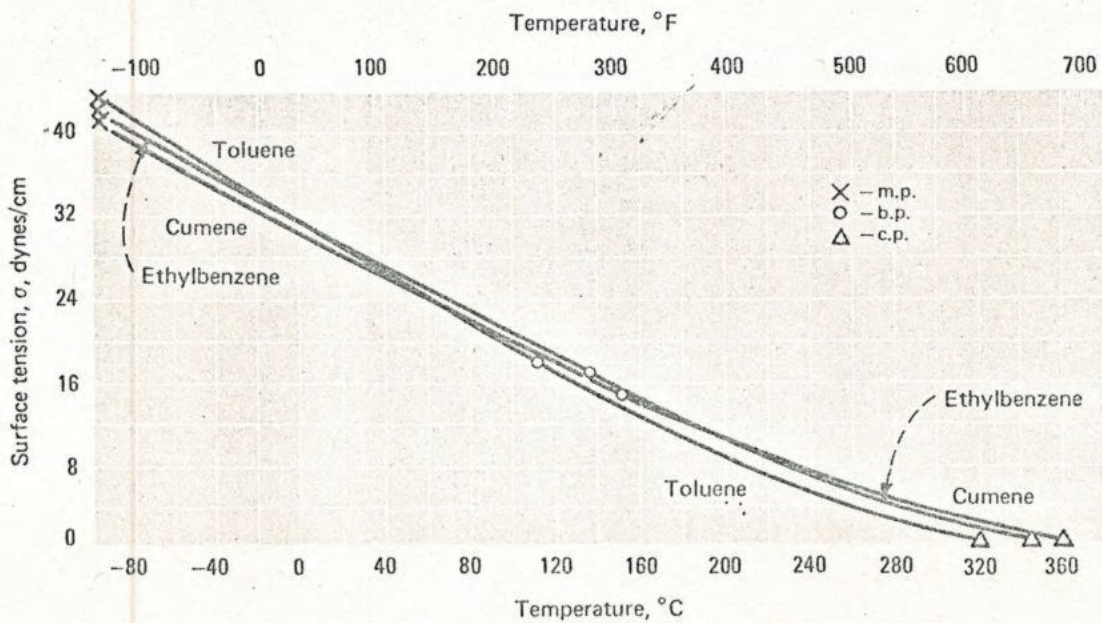
Liquid heat capacity			
Fig. 14-4	Temperature range, C		References
	m.p.-b.p.	b.p.-c.p.	
Toluene	☑	☑	3,19,415,518
Ethylbenzene	☑	☐	9,415
Cumene	☐	☐	14,543

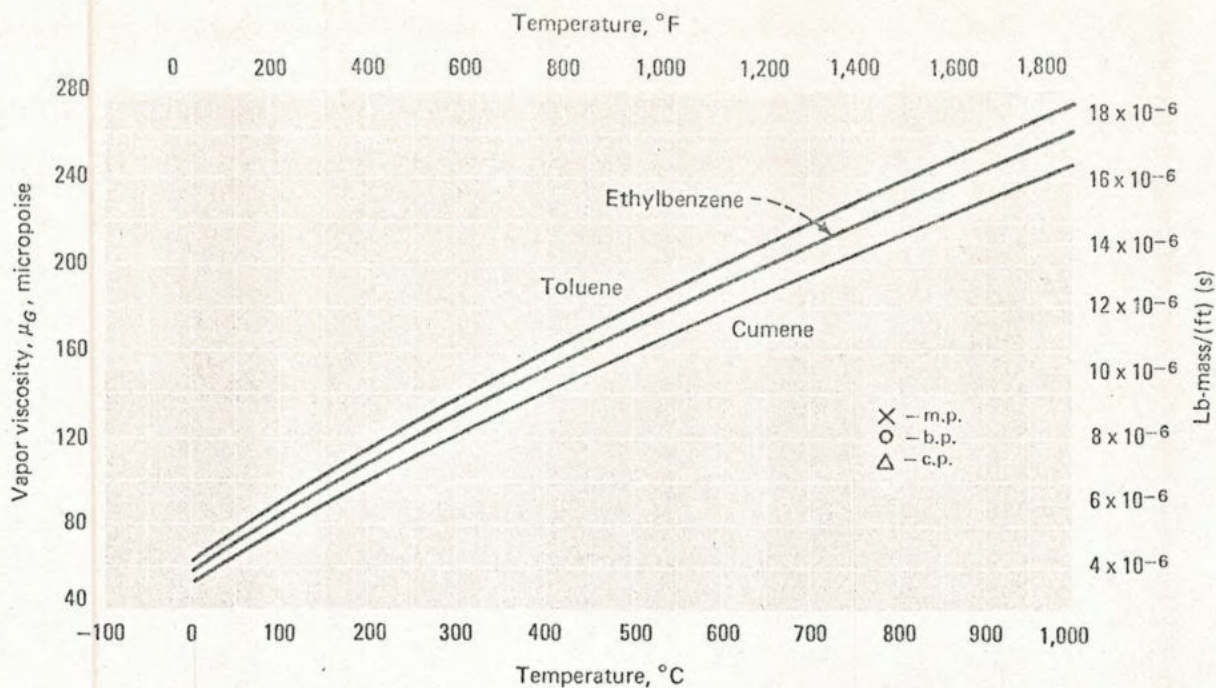




Liquid density			References
Fig. 14-5	Temperature range, °C		
	m.p. - b.p.	b.p. - c.p.	
Toluene	☒	☒	3, 4, 15, 417, 473, 474, 516, 524
Ethylbenzene	☒	☒	3, 4, 15, 417, 473, 474, 516, 524
Cumene	☒	☒	3, 4, 15, 417, 473, 474, 516, 524

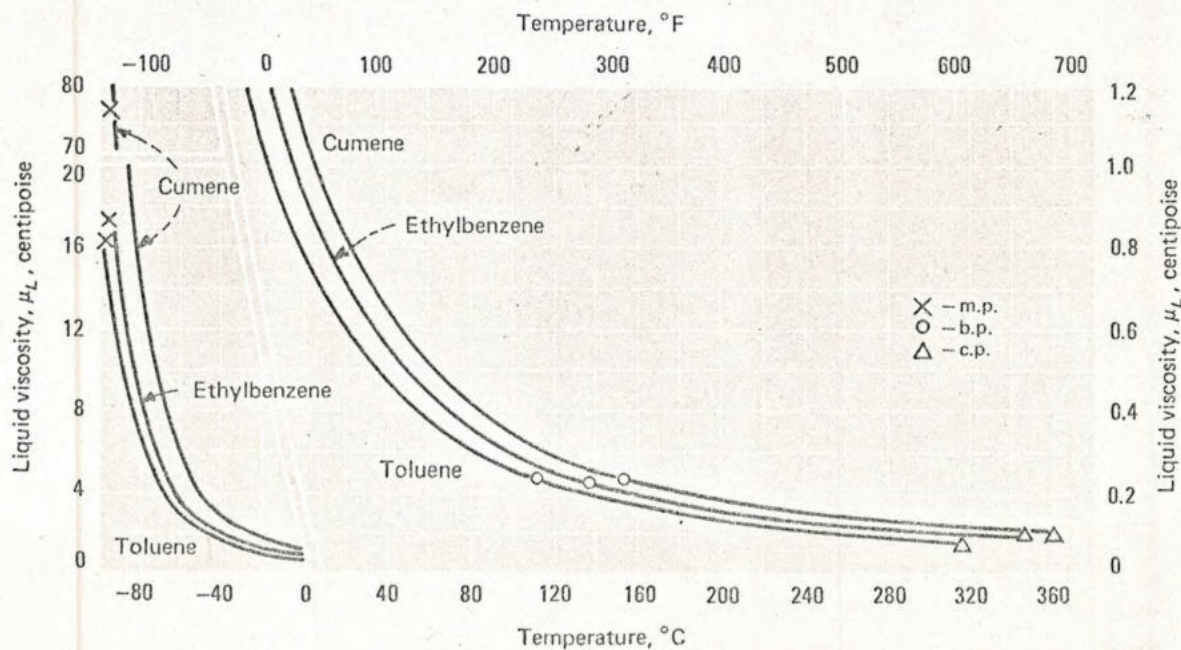
Surface tension			References
Fig. 14-6	Temperature range, °C		
	m.p. - b.p.	b.p. - c.p.	
Toluene	☒	☐	3, 9, 79, 415, 417, 520
Ethylbenzene	☒	☐	3, 9, 79, 415, 417, 520
Cumene	☒	☐	3, 9, 79, 415, 417, 520

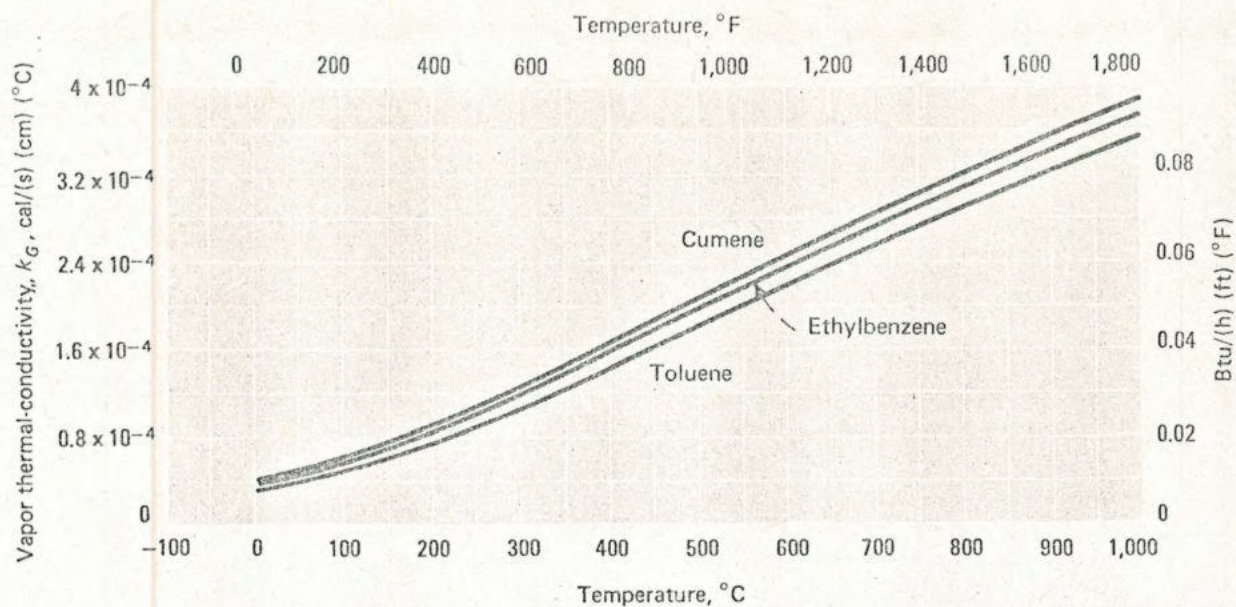




Vapor viscosity			
Fig. 14-7	Temperature range, °C		References
	0-500	500-1,000	
	Toluene	<input checked="" type="checkbox"/>	
Ethylbenzene	<input type="checkbox"/>	<input type="checkbox"/>	442
Cumene	<input type="checkbox"/>	<input type="checkbox"/>	442

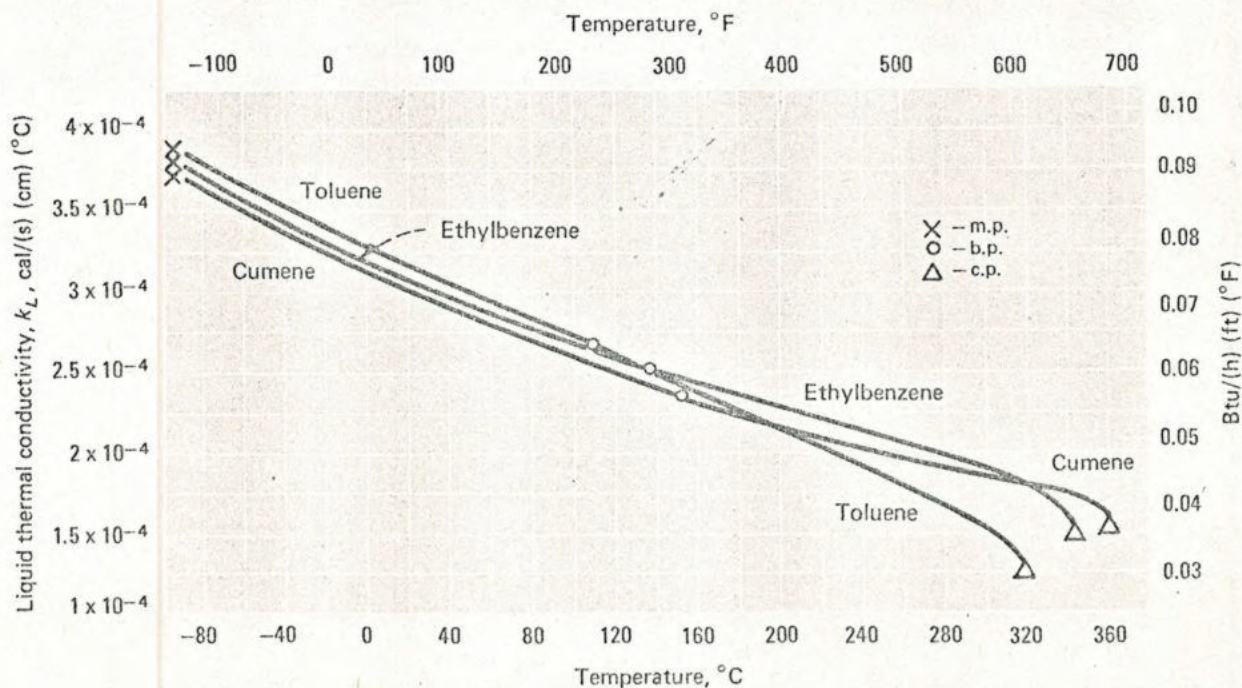
Liquid viscosity			
Fig. 14-8	Temperature range, °C		References
	m.p.-b.p.	b.p.-c.p.	
	Toluene	<input checked="" type="checkbox"/>	
Ethylbenzene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	9, 415, 417, 515, 519, 522, 524, 546
Cumene	<input checked="" type="checkbox"/>	<input type="checkbox"/>	417, 517, 521, 524, 546

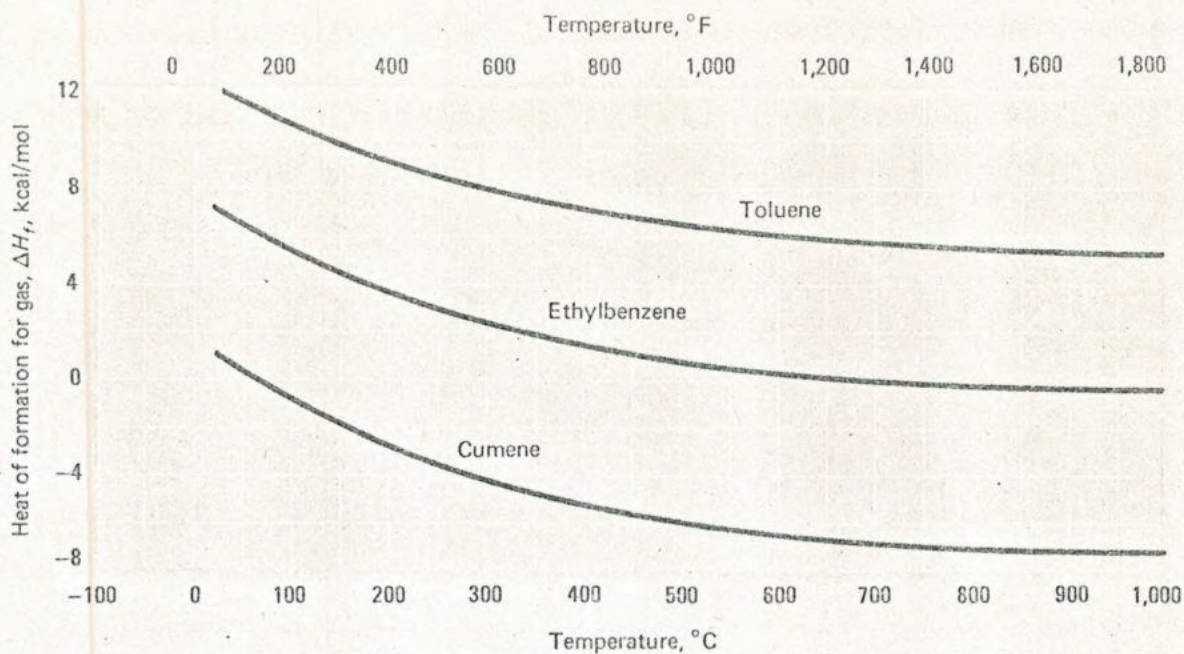




Vapor thermal conductivity			References
Fig. 14-9	Temperature range, $^{\circ}$ C		
	0-500	500-1,000	
Toluene	<input checked="" type="checkbox"/>	<input type="checkbox"/>	19,470,471,494
Ethylbenzene	<input type="checkbox"/>	<input type="checkbox"/>	14,443
Cumene	<input type="checkbox"/>	<input type="checkbox"/>	14,443

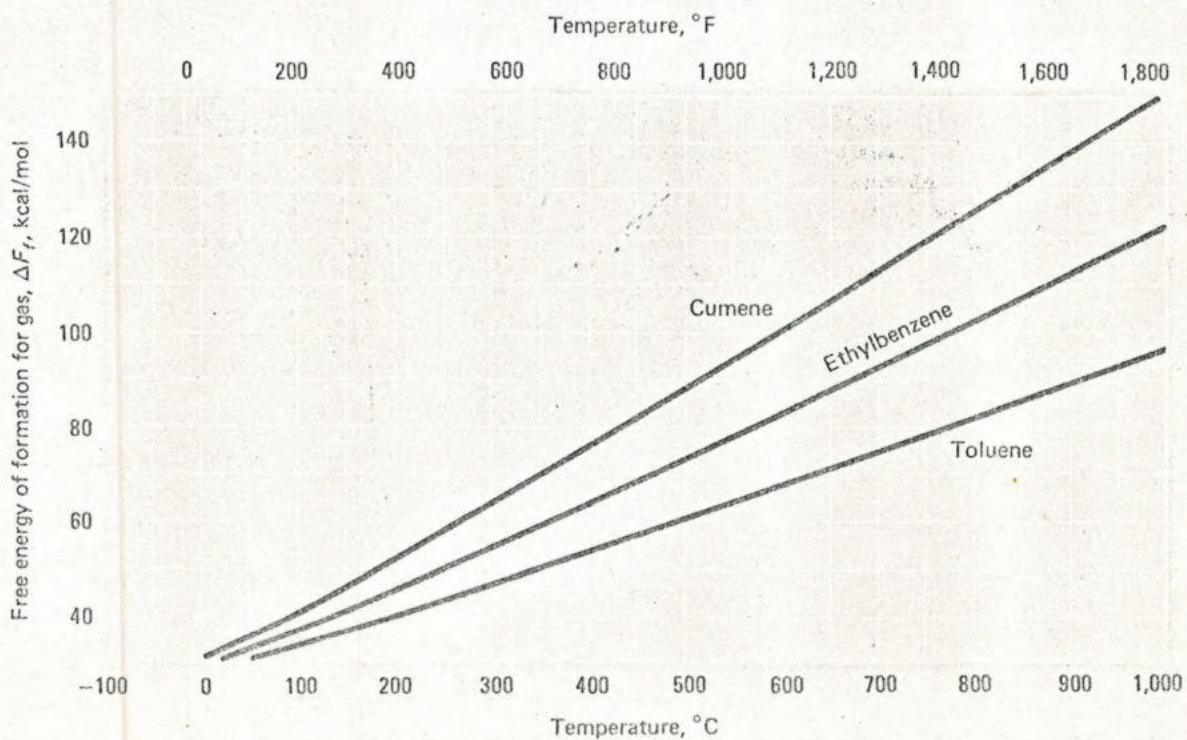
Liquid thermal conductivity			References
Fig. 14-10	Temperature range, $^{\circ}$ C		
	m.p.-b.p.	b.p.-c.p.	
Toluene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	9,14,19,288,409,470,471,475,481,482,483,486,496,516,525,526,527,528,530,531,535,538,539,546
Ethylbenzene	<input checked="" type="checkbox"/>	<input type="checkbox"/>	14,481,516,535,539
Cumene	<input checked="" type="checkbox"/>	<input type="checkbox"/>	14,483,486,516,532,546





Heat of formation for gas			
Fig. 14-11	Temperature range, C		References
	0-500	500-1,000	
Toluene	☑	☑	15,417
Ethylbenzene	☑	☑	15,417
Cumene	☑	☑	15,417

Free energy of formation for gas			
Fig. 14-12	Temperature range, C		References
	0-500	500-1,000	
Toluene	☑	☑	15,417
Ethylbenzene	☑	☑	15,417
Cumene	☑	☑	15,417



results from the relation and the experimental data were 2.6% and 3.2%, respectively, for toluene and ethylbenzene.

Density—F/14—5

The modified Rackett correlation (Eq. 13—1) was selected for extending density data to cover the complete liquid phase. The correlation values agree excellently with the experimental data. Average deviations were only 0.4%, 0.5% and 0.35%, respectively, for toluene, ethylbenzene and cumene.

Surface Tension—F/14—6

Surface-tension data for each alkyl aromatic were correlated with the Othmer relation (Eq. 1—4). The correlation results and data agreed excellently. Average deviations were less than 0.4%.

Viscosity—F/14—7, 14—8

Gas-viscosity data at atmospheric pressure for toluene were extended with the Flynn and Thodos correlation (Eq. 10—1) for hydrocarbon gases. Gas viscosities for ethylbenzene and cumene were also estimated with this modified correlation. The results agree closely with experimental data, with an average deviation of 1.2% for toluene.

Liquid-viscosity data were extended with the Guzman-Andrade relation (Eq. 1—6) for log viscosity vs. reciprocal temperature. Two straight lines fitted the data for each alkyl aromatic. Deviations between the Guzman-Andrade relation and the data averaged 2%, 1.5% and 2.6%, respectively, for toluene, ethylbenzene and cumene.

Thermal Conductivity—F/14—9, F/14—10

The Misic and Thodos correlation (Eq. 12—2a and 12—2b) for hydrocarbon gases at atmospheric pressure was modified for extending the experimental, gas-phase, thermal-conductivity data for toluene. The modified correlation was also effectively applied to estimate gas-phase thermal conductivities of ethylbenzene and cumene. Average deviations of modified correlation

values and experimental data were 6.8% for toluene. Other estimation methods produced considerably larger errors.

Thermal-conductivity data for the saturated liquid of each alkyl aromatic were extended with the modified Stiel and Thodos relation (Eq. 10—3). Values from the relation and experimental data agreed closely. Average deviations were 4.1%, 2.2% and 1%, respectively, for toluene, ethylbenzene and cumene.

Heat and Free Energy of Formation—F/14—11, F/14—12

Results for heat and Gibbs' free energy of formation for the ideal gas are in close agreement. Variations are less than 0.2 kcal/mol for toluene, and 0.01 kcal/mol for ethylbenzene and cumene.

Prior Parts of the Series

This article on toluene, ethylbenzene and cumene—14th part of the series on the physical and thermodynamic properties of industrially important chemicals—has been preceded by the following ones, published on the dates indicated:

Part 1 (June 10, 1974): Halogens (Cl₂, Br₂, F₂, I₂)

Part 2 (July 8, 1974): Sulfur oxides (SO₂, SO₃)

Part 3 (Aug. 19, 1974): Nitrogen oxides (N₂O, NO, NO₂)

Part 4 (Sept. 30, 1974): Carbon oxides (CO, CO₂)

Part 5 (Oct. 26, 1974): Halogen acids (HCl, HF, HBr, HI)

Part 6 (Nov. 25, 1974): Ammonia and hydrazine

Part 7 (Dec. 23, 1974): Water and hydrogen peroxide

Part 8 (Jan. 20, 1975): Diatomic gases (H₂, N₂, O₂)

Part 9 (Feb. 17, 1975): Helium, neon and argon

Part 10 (Mar. 31, 1975): Olefins (C₂H₄, C₃H₆, 1-C₄H₈)

Part 11 (May 12, 1975): Alkanes: CH₄, C₂H₆, C₃H₈

Part 12 (July 21, 1975): Xylenes: ortho, meta, para

Part 13 (Sept. 1, 1975): Benzene and naphthalene

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