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VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

Aromatic Hydrocarbons



Chemistry Data Series

Vol. I, Part 7

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Vapor-Liquid Equilibrium Data Collection

7

Aromatic Hydrocarbons

Tables and diagrams of data for binary and multicomponent mixtures up to moderate pressures.
Constants of correlation equations for computer use.

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7

Aromatic Hydrocarbons

Systems with:

Benzene	Propylbenzene
Toluene	1,2,3-Trimethylbenzene
Styrene	1,2,4-Trimethylbenzene
Ethylbenzene	1,3,5-Trimethylbenzene
m-Xylene	Butylbenzene
o-Xylene	p-Cymene
p-Xylene	1-Methylnaphthalene
Isopropylbenzene	Anthracene

SUBJECTS OF VOLUME I

The table lists the parts of Volume I already published or in preparation.

Subtitle	Vol. I, Part
Aqueous Systems	1 (1980)
Supplement 1	1a (1981)
Supplement 2	1b (1988)
Organic Hydroxy Compounds	
Alcohols	2a (1977)
Alcohols and Phenols	2b (1978)
Supplement 1	2c (1982)
Supplement 2	2d (1982)
Supplement 3	2e (1988)
Supplement 4	2f (1990)
Aldehydes, Ketones, Ethers	3/4 (1979)
Supplement 1, Aldehydes	3a (1993)
Supplement 1, Ketones	3b (1993)
Supplement 1, Ethers	4a (1994)
Carboxylic Acids, Anhydrides, Esters	5 (1982)
Supplement 1	5a (in prep.)
Aliphatic Hydrocarbons C ₄ -C ₆	6a (1980)
Aliphatic Hydrocarbons C ₇ -C ₁₈	6b (1980)
Supplement 1	6c (1984)
Supplement 2	6d (in prep.)
Aromatic Hydrocarbons	7 (1980)
Supplement 1	7a (in prep.)
Halogen, Nitrogen, Sulfur and other Compounds	8 (1984)
Supplement 1	8a (in prep.)

AUTHORS' PREFACE

With part 7 of our Vapor-Liquid Equilibrium Data Collection appearing now, only parts 5 and 8 are still to be completed. Besides, preparation of supplements to parts 1 and 2 has been started. On the whole, we can state to-day, that the amount of work necessary to transform our computerized Dortmund Data Bank (DDB) of vapor-liquid equilibrium data into this printed edition was underestimated by us at the start. So much the more are we indebted to the great number of people who have helped us in various ways. At this point we wish to thank in particular the head of the computer center of the University of Dortmund, Dipl.-Phys. G. Schwichtenberg, and his staff, especially Mr. T. Blaszyk, for their constant co-operation. Likewise we should like to express our gratitude to Dr. R. Eckermann and Chem.-Ing. (grad.) C. Hammer (both DECHEMA, Frankfurt/M.) for their efforts in editing the data collection.

Finally, we should like to mention with thanks all members of our team who were engaged in the preparation of part 7 of our VLE Data Collection; these are: Mrs. U. Arlt, Mrs. A. Brunk, Dipl.-Ing. P. Grenzheuser, Mrs. G. Hennig, Dipl.-Ing. B. Kolbe, Mrs. L. Kunzner, Dr. G. Noçon, Mrs. G. Obermann.

As to the contents of the data sheets, an alteration concerning pure component vapor pressures is to be mentioned here. From this part 7 onwards, including part 5, the vapor pressures of the pure components from the original VLE data publications are used for data evaluation and parameter fitting, wherever such data are reported in the original VLE data set. For this purpose the first Antoine constant (A) is fitted to these pure component vapor pressures, with the two other Antoine constants B and C being taken from our data files for pure compounds, as explained in the General Remarks and Explanations (part 1, p. XXXIX). In case of the Antoine constant A being fitted in this way, it is given at the bottom of the respective data sheet.

Dortmund, August 1980

Ulfert Onken

Jürgen Gmeling

Wolfgang Arlt

PREFACE OF EDITORS

Subjects of this series are the physical and thermodynamic property data of chemical compounds and mixtures essentially for the fluid state covering PVT data, heat capacity, enthalpy, and entropy data, phase equilibrium data, transport and interfacial tension data.

The main purpose is to provide chemists and engineers with data for process design and development. For computer based calculations in process design appropriate correlation methods and accurate data must be used. These are only in some cases available in the open literature. For that reason the most urgent requirement regarding the publication of data is to offer classified and critically evaluated data, thus giving an impression which of them are reliable or not. This will be the goal of the series.

DECHEMA gives the opportunity to authors especially from universities to publish not only their theoretical results, but also their measured or compiled data, most often a large amount, that would otherwise never have been published.

The work of Dr. Gmehling, Prof. Onken and Dipl.-Chem. Arlt on vapor-liquid equilibria which was partly supported by the Federal Ministry of Research and Technology and DECHEMA has been very fruitful; in particular, it led to an extension of the UNIFAC method. The authors have produced what is probably the largest collection of vapor-liquid equilibrium data that is today available with evaluation programs and experimental data.

We present the evaluation of this material in several parts of the first volume of the series. We hope that this gives particularly the users an instrument that will allow them to solve their problems considerably more easily and quickly than before.

Frankfurt/Main, August 1980

Dieter Behrens
Reiner Eckermann

CONTENTS
Vol. I, Part 7

Subjects of Volumes I	VI
Authors' Preface	VII
Preface of Editors	VIII
Contents Volume I, Part 7	IX
Contents Volume I, Part 1	XI
Contents Volume I, Part 2a	XII
Contents Volume I, Part 2b	XIII
Contents Volume I, Parts 3+4	XV
Contents Volume I, Part 6a	XVII
Contents Volume I, Part 6b	XIX
Guide to Tables	XXI
List of Symbols	XXXI
References	XXXIII
Data Tables	1
Binary Systems	1
Benzene	1
Toluene	329
Styrene	445
Ethylbenzene	458
m-Xylene	478
o-Xylene	486
p-Xylene	494
Isopropylbenzene	510
Propylbenzene	511
1,2,3-Trimethylbenzene	512
1,2,4-Trimethylbenzene	520
1,3,5-Trimethylbenzene	524
Butylbenzene	527
p-Cymene	528
1-Methylnaphthalene	530
Anthracene	536

Ternary Systems	537
Benzene	537
Toluene	540
1,2,3-Trimethylbenzene	541
Quaternary Systems	543
Benzene	543
Toluene	544
Appendix A: Pure Component Parameters	547
Formula Index of Systems	553
Alphabetical Index of Systems	559

Formula Index of Systems

R = RECOMMENDED VALUES

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	4TH COMPONENT	PAGE
C ₆ H ₆	BENZENE			
CCL ₂ O	PHOSGENE			1
CCL ₄	TETRACHLOROMETHANE			2- 58 58 R
C ₂ H ₃ N	ACETONITRILE			537-538
CH ₂ Br ₃	TRIBROMOMETHANE			59- 61
CHClF ₂	DIFLUOROCHLOROMETHANE			62- 63
CHCl ₃	CHLOROFORM			64- 83
CH ₃ I	METHYL IODIDE			84
CH ₃ NO ₂	NITROMETHANE			85- 88 88 R
CH ₄ S	METHANETHIOL			89
CS ₂	CARBON DISULFIDE			90-101
C ₂ Cl ₃ F ₃	1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE			102-111 111 R
CCL ₄	TETRACHLOROETHYLENE			112
C ₂ HCl ₃	TRICHLOROETHYLENE			113-118 118 R
C ₂ HCl ₅	PENTACHLOROETHANE			119
C ₂ H ₂ Cl ₄	1,1,2,2-TETRACHLOROETHANE			120
C ₂ H ₃ Cl ₃	1,1,1-TRICHLOROETHANE			121
C ₂ H ₃ N	ACETONITRILE			122-133 133 R
C ₂ H ₄ Br ₂	1,2-DIBROMOETHANE			134-137
C ₂ H ₄ Cl ₂	1,2-DICHLOROETHANE			138-158 158 R
C ₂ H ₅ Br	ETHYL BROMIDE			159
C ₂ H ₅ I	ETHYL IODIDE			160
C ₂ H ₅ NO	N-METHYLFORMAMIDE			161-162
C ₂ H ₅ NO ₂	NITROETHANE			163
C ₂ H ₅ OS	DIMETHYLSULFIDE			164-159
C ₂ H ₅ N ₂	ETHYLENEDIAMINE			170-176
C ₃ H ₃ F ₆ O	1,1,1,3,3,3-HEXAFLUORO-2-PROPANOL			177
C ₃ H ₇ NO	N,N-DIMETHYLFORMAMIDE			178-184 184 R
C ₃ H ₇ NO ₂	1-NITROPROPANE			185
C ₃ H ₇ NO ₂	2-NITROPROPANE			186
C ₃ H ₉ BO ₃	METHYL BORATE			187
C ₄ H ₄ S	THIOPHENE			188-180
C ₄ H ₈ O ₂ S	SULFOLANE			190-191
C ₄ H ₈ O ₂ S	1,4-THIOPHANE-S-OXIDE			192-193

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	4TH COMPONENT	PAGE
C ₃ H ₆	BENZENE			
C ₄ H ₉ NO	METHYL ETHYL KETOXIM			194-198 198 P
C ₄ H ₁₁ N	BUTYLAMINE			199-201 201 R
C ₄ H ₁₁ N	TERT-BUTYLAMINE			202-204
C ₄ H ₁₁ N	DIETHYLAMINE			205-207
C ₅ H ₅ N	PYRIDINE			208-221
C ₅ H ₁₁ NO	DIETHYLFORMAMIDE			222-225 225 R
C ₆ F ₆	HEXAFLUOROBENZENE			226-237 237 P
C ₆ H ₄ Cl ₂	P-DICHLOROBENZENE			238
C ₆ H ₅ Br	BROMOBENZENE			239-242
C ₆ H ₅ Cl	CHLOROBENZENE			243-251 251 R
C ₆ H ₅ F	FLUOROBENZENE			252
C ₆ H ₅ NO ₂	NITROBENZENE			253-254
C ₆ H ₇ N	ANILINE			255-266 266 R
C ₆ H ₁₁ Cl	CHLOROCYCLOHEXANE			267-270
C ₆ H ₁₁ NO	6-CAPROLACTAM			271
C ₆ H ₁₃ N	CYCLOHEXYLAMINE			272-274
C ₆ H ₁₅ N	TRIETHYLAMINE			275-277 277 R
C ₇ H ₅ N	BENZONITRILE			278
C ₇ H ₈	TOLUENE			279-301 301 R
C ₇ H ₁₅ N	N-METHYLCYCLOHEXYLAMINE	C ₈ H ₁₀	ETHYLBENZENE	302-304 304 R
C ₈ H ₈	STYRENE	C ₉ H ₁₀	ALPHA-METHYLSTYRENE	305
C ₈ H ₁₀	ETHYLBENZENE	C ₉ H ₁₂	ISOPROPYLBENZENE	306
C ₈ H ₁₂	M-XYLENE			307-309
C ₈ H ₁₂	P-XYLENE			310-311
C ₈ H ₁₁ N	N,N-DIMETHYLANILINE			312
C ₈ H ₂₀ S ₁	TETRAETHYL SILANE			313-316 316 P
C ₉ H ₂₄ O ₄ S ₁	OCTAMETHYLCLOTETRAISILOXANE			317-321
C ₉ H ₁₂	ISOPROPYLBENZENE			322
C ₉ H ₁₂	PROPYLBENZENE			323
C ₁₀ H ₁₄	BIPHENYL			324-326
C ₁₀ H ₁₄	N-TERPHENYL			327-328

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	4TH COMPONENT	PAGE
C ₇ H ₁₃	TOLUENE			
CCL ₄	TETRACHLOROMETHANE			329-351 351 R
CHCl ₃	CHLOROFORM	C ₂ H ₄ Br ₂	1,2-DIBROMOETHANE	354
C ₂ S ₂	CARBON DISULFIDE			354-361
C ₂ HCl ₃	TRICHLOROETHYLENE			362-371
C ₂ H ₃ N	ACETONITRILE			372-375
C ₂ H ₃ NO	METHYL ISOCYANATE			376
C ₂ H ₄ Cl ₂	1,2-DICHLOROETHANE			377-384 384 R
C ₂ H ₅ NO ₂	NITROETHANE			385
C ₂ H ₆ S	DIMETHYLSULFOXIDE			386
C ₂ H ₈ N ₂	ETHYLENEDIAMINE			387
C ₃ H ₅ N	PROPIONITRILE			388-389
C ₃ H ₇ NO	N,N-DIMETHYLFORMAMIDE			390-394
C ₄ H ₆ S	THIOPHENE			395-396
C ₄ H ₇ N	BUTYRONITRILE			397
C ₄ H ₈ O ₂ S	SULFOLANE			398-399
C ₄ H ₁₁ N	DIETHYLAMINE			400
C ₅ H ₅ N	PYRIDINE			401-407
C ₅ F ₆	HEXAFLUOROBENZENE			408-414 414 R
C ₆ H ₅ Br	BROMOBENZENE			415
C ₆ H ₅ Cl	CHLOROBENZENE			416-417
C ₆ H ₅ F	FLUOROBENZENE			418-421 421 R
C ₆ H ₅ NO ₂	NITROBENZENE			422
C ₆ H ₇ N	ANILINE			423-431 431 R
C ₆ H ₇ N	2-METHYLPYRIDINE			432
C ₆ H ₇ N	3-METHYLPYRIDINE			433
C ₆ H ₁₁ NO	6-CAPROLACTAM			434
C ₇ H ₅ N	BENZONITRILE			435
C ₇ H ₇ F	O-FLUOROTOLUENE			436-439
C ₇ H ₂₂ O ₂ S ₁₃	1,1,1,3,5,5,5-HEPTAMETHYLTRISILOXANE			440-442
C ₈ H ₁₀	ETHYLBENZENE	C ₉ H ₁₀	ALPHA-METHYLSTYRENE	443
		C ₉ H ₁₂	ISOPROPYLBENZENE	544
C ₈ H ₁₀	P-XYLENE			444
C ₈ H ₈	STYRENE			
C ₂ HCl ₅	PENTACHLOROETHANE			445

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
		4TH COMPONENT	
=====			
C ₃ H ₃	STYRENE		
=====			
C ₃ H ₃ N	ACRYLONITRILE		446
C ₃ H ₁₀	ETHYLBENZENE		447-455
C ₉ H ₁₀	ALPHA-METHYLSTYRENE		456
C ₉ H ₁₂	PROPYLBENZENE		457
=====			
C ₃ H ₁₀ ETHYLBENZENE			
=====			
CCL ₄	TETRACHLOROMETHANE		458-464
C ₃ H ₃ N	ACETONITRILE		465
C ₂ H ₄ Cl ₂	1,2-DICHLOROETHANE		466
C ₃ H ₃ N	ACRYLONITRILE		467
C ₄ H ₁₁ N	DIETHYLAMINE		468
C ₆ H ₅ Cl	CHLOROBENZENE		469
C ₆ H ₅ N ₂	NITROBENZENE		470
C ₆ H ₇ N	ANILINE		471-475 475 R
=====			
C ₉ H ₁₂	ISOPROPYLBENZENE		476
C ₁₀ H ₁₄	BUTYLBENZENE		477
=====			
C ₈ H ₁₀ M-XYLENE			
=====			
CCL ₄	TETRACHLOROMETHANE		478-480
C ₃ H ₇ NO	N,N-DIMETHYLFORMAMIDE		481
C ₅ H ₅ N	PYRIDINE		482
C ₆ H ₇ N	ANILINE		483
C ₈ H ₁₀	P-XYLENE		484-485
=====			
C ₈ H ₁₀ O-XYLENE			
=====			
CCL ₄	TETRACHLOROMETHANE		486-488
C ₂ H ₅ Cl ₅	PENTACHLOROETHANE		489
C ₂ H ₄ Cl ₂	1,2-DICHLOROETHANE		490
C ₂ H ₈ N ₂	ETHYLENEDIAMINE		491-492
C ₃ H ₇ NO	N,N-DIMETHYLFORMAMIDE		493
=====			
C ₈ H ₁₀ P-XYLENE			
=====			
CCL ₂ O	PHOSGENE		494-495
CCL ₄	TETRACHLOROMETHANE		496-498
C ₃ H ₃ N	ACETONITRILE		499
C ₂ H ₄ Cl ₂	1,2-DICHLOROETHANE		500
C ₃ H ₇ NO	N,N-DIMETHYLFORMAMIDE		501
C ₆ F ₆	HEXAFLUOROBENZENE		502-507 507 R
=====			

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
		4TH COMPONENT	
C ₃ H ₁₀	P-XYLENE		
	C ₆ H ₅ CL CHLOROBENZENE		508
	C ₆ H ₇ N ANILINE		509
C ₉ H ₁₂	ISOPROPYLBENZENE		
	CCL ₄ TETRACHLOROMETHANE		510
C ₉ H ₁₂	PROPYLBENZENE		
	C ₆ H ₅ NO ₂ NITROBENZENE		511
C ₉ H ₁₂	1,2,3-TRIMETHYLBENZENE		
	C ₉ H ₁₂ 1,2,4-TRIMETHYLBENZENE		512-515
		C ₉ H ₁₂ 1,3,5-TRIMETHYLBENZENE	541-542
	C ₉ H ₁₂ 1,3,5-TRIMETHYLBENZENE		516-519
C ₉ H ₁₂	1,2,4-TRIMETHYLBENZENE		
	C ₉ H ₁₂ 1,3,5-TRIMETHYLBENZENE		520-523
C ₉ H ₁₂	1,3,5-TRIMETHYLBENZENE		
	C ₆ H ₁₅ N TRIETHYLAMINE		524-526
C ₁₀ H ₁₄	BUTYLBENZENE		
	C ₆ H ₅ NO ₂ NITROBENZENE		527
C ₁₀ H ₁₄	P-CYMENE		
	C ₆ H ₇ N ANILINE		528-529
C ₁₁ H ₁₀	1-METHYLNAPHTHALENE		
	C ₁₁ H ₁₀ 2-METHYLNAPHTHALENE		530-535
C ₁₄ H ₁₀	ANTHRACENE		
	C ₁₄ H ₁₀ PHENANTHRENE		536

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
		4TH COMPONENT	
ANTHRACENE	C14H10		
	PHENANTHRENE	C14H10	536
RENZENE	C6H6		
	ACETONITRILE	C2H3N	122-133 133 R
	ANILINE	C6H7N	255-266 266 R
	BENZONITRILE	C7H5N	278
	BIPHENYL	C12H10	324-326
	BROMOBENZENE	C6H5BR	239-242
	BUTYLAMINE	C4H11N	199-201 201 R
TERT-BUTYLAMINE	C6H11N		202-204
6-CAPROLACTAM	C6H11NO		271
CARBON DISULFIDE	CS2		90-101
CHLOROBENZENE	C6H5CL		243-251 251 R
CHLOROCYCLOHEXANE	C6H11CL		267-270
CHLORFORM	CHCL3		64- 83
CYCLOCHEXYLAMINE	C6H13N		272-274
1,2-DIBROMOETHANE	C2H4BR2		134-137
P-DICHLOROBENZENE	C6H4CL2		238
1,2-DICHLOROETHANE	C2H4CL2		138-158 158 R
DIETHYLAMINE	C4H11N		205-207
DIETHYLFORMAMIDE	C5H11NO		222-225 225 R
DIFLUOROCHLOROMETHANE	CHCLF2		62- 63
N,N-DIMETHYLANILINE	C8H11N		312
N,N-DIMETHYLFORMAMIDE	C3H7NO		178-184 184 R
DIMETHYLSULFOXIDE	C2H6OS		164-169
ETHYLBENZENE	C8H10		306
	ISOPROPYLBENZENE	C9H12	
	ALPHA-METHYLSTYRENE	C9H10	543
ETHYL BROMIDE	C2H5BR		159
ETHYLENEDIAMINE	C2H8N2		170-176
ETHYL IODIDE	C2H5I		160
FLUOROBENZENE	C6H5F		252
HEXAFLUOROBENZENE	C6F6		226-237 237 R
1,1,1,3,3,3-HEXAFLUORO-2-PROPANOL	C3H2F6O		177
	ISOPROPYLBENZENE	C9H12	322
METHANETHIOL	CH4S		89

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE
BENZENE	C6H6		
METHYL BORATE	C3H9B03		187
N-METHYL CYCLOHEXYLAMINE	C7H15N		302-304 304 R
METHYL ETHYL KETOXIM	C4H9NO		194-198 198 R
N-METHYLFORMAMIDE	C2H5NO		161-162
METHYL IODIDE	CH3I		84
NITROBENZENE	C6H5NO2		253-254
NITROETHANE	C2H5NO2		163
NITROMETHANE	CH3NO2		85- 88 88 R
1-NITROPROPANE	C3H7NO2		185
2-NITROPROPANE	C3H7NO2		186
OCTAMETHYL- CYCLOTETRASILOXANE	C8H24O4Si4		317-321
PENTACHLOROETHANE	C2HCl5		119
PHOSGENE	CCL2O		1
PROPYLBENZENE	C9H12		323
PYRIDINE	C5H5N		208-221
STYRENE	C8H8		305
SULFOLANE	C4H8O2S		190-191
P-TERPHENYL	C18H14		327-328
1,1,2,2-TETRACHLOROETHANE	C2H2Cl4		120
TETRACHLOROETHYLENE	C2Cl4		112
TETRACHLORMETHANE	CCL4		2- 58 58 R
	ACETONITRILE	C2H3N	537-538
TETRAETHYL SILANE	C8H20Si		313-316 316 R
THIOPHENE	C4H4S		188-189
1,4-THIOXANE-S-OXIDE	C4H8O2S		192-193
TOLUENE	C7H8		279-301 301 R
	ETHYLBENZENE	C8H10	539
TRIBROMOMETHANE	CHBr3		59- 61
1,1,1-TRICHLOROETHANE	C2H3Cl3		121
TRICHLOROETHYLENE	C2HCl3		113-118 118 R
1,1,2-TRICHLORO-1,2,2- TRIFLUOROETHANE	C2Cl3F3		102-111 111 R
TRIETHYLAMINE	C6H15N		275-277 277 R
M-XYLENE	C8H10		307-309
P-XYLENE	C8H10		310-311

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE
BUTYLBENZENE	C10H14		
	NITROBENZENE	C6H5NO2	527
P-CYMENE	C10H14		
	ANILINE	C6H7N	528-529
ETHYLBENZENE	C8H10		
	ACETONITRILE	C2H3N	465
	ACRYLONITRILE	C3H3N	467
	ANILINE	C6H7N	471-475 475 R
	BUTYLBENZENE	C10H14	477
	CHLOROBENZENE	C6H5CL	469
1,2-DICHLOROETHANE	C2H4CL2		466
	DIETHYLAMINE	C6H11N	468
	ISOPROPYLBENZENE	C9H12	476
	NITROBENZENE	C6H5NO2	470
	TETRACHLOROMETHANE	CCL4	458-464
ISOPROPYLBENZENE	C9H12		
	TETRACHLOROMETHANE	CCL4	510
1-METHYLNAPHTHALENE	C11H10		
	2-METHYLNAPHTHALENE	C11H10	530-535
PROPYLBENZENE	C9H12		
	NITROBENZENE	C6H5NO2	511
STYRENE	C8H8		
	ACRYLONITRILE	C3H3N	446
	ETHYLBENZENE	C8H10	447-455
	ALPHA-METHYLSTYRENE	C9H10	456
	PENTACHLOROETHANE	C2HCL5	445
	PROPYLBENZENE	C9H12	457
TOLUENE	C7H8		
	ACETONITRILE	C2H3N	372-375
	ANILINE	C6H7N	423-431 431 R
	BENZONITRILE	C7H5N	435
	BROMOBENZENE	C6H5BR	415
	BUTYRONITRILE	C4H7N	397

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
		4TH COMPONENT	
TOLUENE	C7H8		
6-CAPROLACTAM	C6H11NO		434
CARBON DISULFIDE	CS2		354-361
CHLOROBENZENE	C6H5CL		416-417
CHLORFORM	CHCl3		352-353
1,2-DICHLOROETHANE	C2H4Cl2		377-384 384 R
DIETHYLAmine	C4H11N		400
N,N-DIMETHYLFORMAMIDE	C3H7NO		390-394
DIMETHYLSULFOXIDE	C2H6OS		386
ETHYLBENZENE	C8H10		443
	ISOPROPYLBENZENE	C9H12	
	ALPHA-METHYLSTYRENE	C9H10	544
ETHYLENEDIAMINE	C2H8N2		387
FLUOROBENZENE	C6H5F		418-421 421 R
C-FLUOROTOLUENE	C7H7F		436-439
1,1,1,3,5,5-HEPTAMETHYL-TRISILOXANE	C7H22O2Si3		440-442
HEXAFLUOROBENZENE	C6F6		408-414 414 R
METHYL ISOCYANATE	C2H3NO		376
2-METHYL PYRIDINE	C6H7N		432
3-METHYL PYRIDINE	C6H7N		433
NITROBENZENE	C6H5NO2		422
NITROETHANE	C2H5NO2		385
PROPIONITRILE	C3H5N		388-389
PYRIDINE	C5H5N		401-407
SULFOLANE	C4H8O2S		398-399
TETRACHLOROMETHANE	CCL4		329-351 351 R
	1,2-DIBROMOETHANE	C2H4Br2	540
THIOPHENE	C4H4S		395-396
TRICHLOROETHYLENE	C2HCl3		362-371
P-XYLENE	C8H10		444
1,2,3-TRIMETHYLBENZENE	C9H12		
1,2,4-TRIMETHYLBENZENE	C9H12		512-515
1,3,5-TRIMETHYLBENZENE	C9H12		541-542
1,2,4-TRIMETHYLBENZENE	C9H12		516-519
1,3,5-TRIMETHYLBENZENE	C9H12		

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
		4TH COMPONENT	
1,3,5-TRIMETHYLBENZENE	C9H12		
	TRIETHYLAMINE	C6H15N	524-526
M-XYLENE	C8H10		
	ANILINE	C6H7N	483
	N,N-DIMETHYLFORMAMIDE	C3H7NO	481
	PYRIDINE	C5H5N	482
	TETRACHLOROMETHANE	CCL4	478-480
	P-XYLENE	C8H10	484-485
O-XYLENE	C8H10		
	1,2-DICHLOROETHANE	C2H4CL2	490
	N,N-DIMETHYLFORMAMIDE	C3H7NO	493
	ETHYLENEDIAMINE	C2H8N2	491-492
	PENTACHLOROETHANE	C2HCL5	489
	TETRACHLOROMETHANE	CCL4	486-488
P-XYLENE	C8H10		
	ACETONITRILE	C2H3N	499
	ANILINE	C6H7N	509
	CHLOROBENZENE	C6H5CL	508
	1,2-DICHLOROETHANE	C2H4CL2	500
	N,N-DIMETHYLFORMAMIDE	C3H7NO	501
	HEXAFLUOROBENZENE	C6F6	502-507 R
	PHOSGENE	CCL2O	494-495
	TETRACHLOROMETHANE	CCL4	496-498