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VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

Aliphatic Hydrocarbons

C₄ – C₆



Chemistry Data Series

Vol. I, Part 6a

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Editors: Dieter Behrens, Reiner Eckermann

Vapor-Liquid Equilibrium Data Collection

6a

Aliphatic Hydrocarbons

C₄–C₆

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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6a

Aliphatic Hydrocarbons

C₄—C₆

Systems with:

1,3-Butadiene	2-Methylbutane
Butane	2-Methyl-1-butene
i-Butene	2-Methyl-2-butene
1-Butene	Methylcyclopentane
Cyclohexane	2-Methylpentane
Cyclohexene	3-Methylpentane
Cyclopentadiene	2-Methyl-1-pentene
Cyclopentane	4-Methyl-1-pentene
2,2-Dimethylbutane	Neopentane
2,3-Dimethylbutane	trans-1,3-Pentadiene
Hexane	Pentane
1-Hexene	1-Pentene
Isoprene	Vinylacetylene

SUBJECTS OF VOLUME I

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

Subtitle	Vol. I, Part
Aqueous-Organic Systems Supplement 1	1 published 1a in prep.
Organic Hydroxy Compounds	
Alcohols	2a published
Alcohols and Phenols	2b published
Supplement 1	2c in prep.
Aldehydes, Ketones, Ethers	3/4 published
Esters and Carboxylic Acids	5 in prep.
Aliphatic Hydrocarbons	6a published 6b published
Aromatic Hydrocarbons	7 in prep.
Halogen, Nitrogen, Sulfur and other Compounds	8 in prep.

AUTHORS' PREFACE

Continuing the publication of our Vapor-Liquid Equilibrium Data Collection we are presenting Part 6, subdivided into Parts 6a and 6b. Completion of Part 5 has been postponed, because in correlating systems containing carboxylic acids we also intend to include vapor phase non-ideality for more than one associating component in a system; programming of this calculation procedure has not yet been finished.

From Part 5 onwards, parameters of activity coefficient equations are also given for "incomplete" x-y data (isothermal without P, resp. isobaric without T). In these cases, equilibrium ratios y/x have been used in the objective function for parameter optimization. A further additional information in the tables from Part 5 onwards concerns incomplete isothermal x-y data; here the result of the consistency test by method 2 (area test of Redlich and Kister) is given.

We again express our thanks to the great number of colleagues who have supported our efforts by supplying VLE data from their laboratories. On this occasion we should like to repeat our plea to all workers in the field of vapor-liquid equilibrium to send us reprints of new experimental results.

Special thanks are due to Dipl.-Phys. G. Schwichtenberg, head of the computer center of the University of Dortmund, and to his staff, especially to H. Förster and U. Liebegut, for their co-operation. We are also grateful to Dr. R. Eckermann (DECHEMA, Frankfurt/M.) for his efforts in editing the data collection.

Finally, we wish to thank all members of our team who helped in the preparation of Part 6 of the VLE Data Collection; these are: Mrs. U. Arlt, Dipl.-Ing. P. Grenzheuser, Miss G. Hennig, W. Kirchhoff, Dipl.-Ing. B. Kolbe, Mrs. S. Koort, Mrs. L. Kunzner, Dr. G. Nocon.

Dortmund, January 1980

Ulfert Onken

Jürgen Gmehling

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 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, January 1980

Dieter Behrens
Reiner Eckermann

CONTENTS
Vol. I, Part 6a

Subjects of Volume I	VI
Authors' Preface	VII
Preface of Editors	VIII
Contents Volume I, Part 6a	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
Guide to Tables	XVII
List of Symbols	XXVII
References	XXIX
Data Tables	1
Binary Systems	1
Vinylacetylene	1
1,3-Butadiene	3
1-Butene	17
Isobutene	18
Butane	19
Cyclopentadiene	36
Isoprene	38
trans-1,3-Pentadiene	57
Cyclopentane	60
2-Methyl-1-butene	77
2-Methyl-2-butene	79
1-Pentene	85
2-Methylbutane	86
Neopentane	90
Pentane	100
Cyclohexene	128
Cyclohexane	139
1-Hexene	340
Methylcyclopentane	361
2-Methyl-1-pentene	376
4-Methyl-1-pentene	378
2,2-Dimethylbutane	381

2,3-Dimethylbutane	387
Hexane	398
2-Methylpentane	619
3-Methylpentane	626
Ternary Systems	631
Cyclopentadiene	631
Isoprene	632
Cyclohexene	634
Cyclohexane	636
1-Hexene	651
Methylcyclopentane	652
Hexane	659
Appendix A: Pure Component Parameters	667
Formula Index of Systems	673
Alphabetical Index of Systems	681

Formula Index of Systems

R-RECOMMENDED VALUES

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE	
C4H4	VINYLCETYLENE			
	C6H6	BENZENE	1	
	C8H10	P-XYLENE	2	
C4H6	1,3-BUTADIENE			
	CCL4	TETRACHLOROMETHANE	3	
	CH2CL2	DICHLOROMETHANE	4	
	CH3NO2	NITROMETHANE	5	
	CS2	CARBON DISULFIDE	6	
	C4H5CL	2-CHLORO-1,3-BUTADIENE	7	
	C4H8	1-BUTENE	8- 10 10 R	
	C4H10	BUTANE	11- 13	
	C6H6	BENZENE	14	
	C8H8	STYRENE	15- 16	
C4H8	1-BUTENE			
	C4H10	BUTANE	17	
C4H8	ISOBUTENE			
	C5H8	ISOPRENE	18	
C4H10	BUTANE			
	CH5N	METHYLAMINE	19- 21	
	C2H5CL	ETHYL CHLORIDE	22	
	C2H5D2N	N-DEUTEROETHYLAMINE	23- 27	
	C2H7N	ETHYLAMINE	28	
	C4F8	PERFLUOROCYCLOBUTANE	29	
	C5H12	PENTANE	30	
	C6H14	HEXANE	31- 35	
C5H6	CYCLOPENTADIENE			
	C5H8	ISOPRENE	36	
		C5H10	2-METHYL-2-BUTENE	631
	C5H10	2-METHYL-2-BUTENE	37	
C5H8	ISOPRENE			
	CH3NO2	NITROMETHANE	38	
	C2H3N	ACETONITRILE	39- 40	
		C5H10	2-METHYL-2-BUTENE	632-633

Formula Index of Systems

=====		
C5H8	ISOPRENE	
C2H6OS	DIMETHYLSULFOXIDE	41 - 43
C3H7NO	N,N-DIMETHYLFORMAMIDE	44
C5H8	TR-1,3-PENTADIENE	45
C5H10	2-METHYL-1-BUTENE	46 - 47
C5H10	2-METHYL-2-BUTENE	48 - 53
C5H10	3-METHYL-1-BUTENE	54 - 55
C5H12	2-METHYLBUTANE	56
=====		
C5H8	TR-1,3-PENTADIENE	
C2H6OS	DIMETHYLSULFOXIDE	57 - 59
=====		
C5H10	CYCLOPENTANE	
CCL4	TETRACHLOROMETHANE	60 - 61
CHCL3	CHLOROFORM	62
CS2	CARBON DISULFIDE	63 - 66 66 R
C2CL4	TETRACHLOROETHYLENE	67
C3HRS	2-PROPANETHIOL	68
C6H6	BENZENE	69 - 73
C6H14	2,3-DIMETHYLBUTANE	74
C10H18	CIS-DECAHYDRONAPHTHALENE	75
C10H18	TRA-DECAHYDRONAPHTHALENE	76
=====		
C5H10	2-METHYL-1-BUTENE	
CH3NO2	NITROMETHANE	77
C5H10	2-METHYL-2-BUTENE	78
=====		
C5H10	2-METHYL-2-BUTENE	
CH3NO2	NITROMETHANE	79
C2H3N	ACETONITRILE	80 - 82
C3H7NO	N,N-DIMETHYLFORMAMIDE	83
C5H12	2-METHYLBUTANE	84
=====		
C5H10	1-PENTENE	
C2H3N	ACETONITRILE	85
=====		
C5H12	2-METHYLBUTANE	
CS2	CARBON DISULFIDE	86 - 87
C2H3N	ACETONITRILE	88
C3H7NO	N,N-DIMETHYLFORMAMIDE	89
=====		

Formula Index of Systems

=====			
C5H12	NEOPENTANE		
C4H12SI	TETRAMETHYLSILANE		90-94
C5H12	PENTANE		95-99
=====			
C5H12	PENTANE		
CH2CL2	DICHLOROMETHANE		100
C2H3N	ACETONITRILE		101-102
C3H3N	ACRYLONITRILE		103-104
C3H8S	1-PROPANETHIOL		105
C5H11BR	PENTYL BROMIDE		106-113
C6H6	BENZENE		114-118
C6H12	CYCLOHEXANE		119
C6H12	METHYLCYCLOHEXANE		120-121
C6H14	HEXANE		122-123
C7H14	METHYLCYCLOHEXANE		124-125
C7H16	HEPTANE		126-127
=====			
C6H10	CYCLOHEXENE		
CCL4	TETRACHLOROMETHANE		128
C2H4CL2	1,2-DICHLOROETHANE		129
		C6H12	CYCLOHEXANE
			634-635
C6H6	BENZENE		130-136
			136 R
C6H12	CYCLOHEXANE		137-138
=====			
C6H12	CYCLOHEXANE		
CCL4	TETRACHLOROMETHANE		139-150
			150 R
CHCLF2	CHLORODIFLUOROMETHANE		151-152
CH3NO2	NITROMETHANE	C6H6	BENZENE
			636
CS2	CARBON DISULFIDE		153-154
C2HCL3	TRICHLOROETHYLENE		155
		C6H6	BENZENE
			637-638
C2HCL5	PENTACHLOROETHANE		156
C2H4BR2	1,2-DIBROMOETHANE		157
C2H4CL2	1,2-DICHLOROETHANE		158-163
			163 R
C2H5NO	N-METHYLFORMAMIDE		164-165
C3H3NS	THIAZOLE		166
C4H4S	THIOPHENE		167
C4H9N	PYRROLIDINE		168-170
			170 R
C5H5N	PYRIDINE		171-182

Formula Index of Systems

C ₆ H ₁₂		CYCLOHEXANE	
C ₅ H ₁₁ N	PIPERIDINE		183-185 185 R
C ₆ F ₆	HEXAFLUOROBENZENE		186-191 191 R
C ₆ F ₁₂	PERFLUOROCYCLOHEXANE		192-195
C ₆ H ₅ BR	BROMOBENZENE		196-201
C ₆ H ₅ CL	CHLOROBENZENE		202
C ₆ H ₅ NO ₂	NITROBENZENE		203
C ₆ H ₆	BENZENE		204-241 240-241 R
		C ₆ H ₇ N	ANILINE 639
		C ₆ H ₁₄	HEXANE 640-647
		C ₇ H ₈	TOLUENE 648
C ₆ H ₇ N	ANILINE		242-257 257 R
C ₆ H ₁₁ CL	CHLOROCYCLOHEXANE		258-261
C ₆ H ₁₂	METHYLCYCLOPENTANE		262
C ₆ H ₁₃ N	CYCLOHEXYLAMINE		263-269
C ₆ H ₁₃ N	HEXAMETHYLENIMINE		270-271
C ₆ H ₁₄	DIMETHYLBUTANE		272
C ₆ H ₁₄	HEXANE		273-277 277 R
C ₇ H ₈	TOLUENE		278-291
		C ₇ H ₁₆	HEPTANE 649-650
C ₇ H ₉ N	METHYLANILINE		292-294
C ₇ H ₁₄	METHYLCYCLOHEXANE		295
C ₇ H ₁₅ N	N-METHYLCYCLOHEXYLAMINE		296-299 299 R
C ₇ H ₁₆	HEPTANE		300-306 306 R
C ₇ H ₁₆	TRIMETHYLBUTANE		307
C ₈ H ₁₀	ETHYLBENZENE		308-310
C ₈ H ₁₀	O-XYLENE		311-312
C ₈ H ₁₀	M-XYLENE		313-314
C ₈ H ₁₀	P-XYLENE		315-318
C ₈ H ₁₆	1-OCTENE		319
C ₈ H ₁₈	OCTANE		320-323
C ₈ H ₁₈	2,2,4-TRIMETHYLPENTANE		324-329 329 R
C ₁₂ H ₂₆	DODECANE		330-333
C ₁₆ H ₃₄	HEXADECANE		334-336
C ₂₀ H ₄₂	EICOSANE		337-339

C₆H₁₂

1-HEXENE

CCL ₄	TETRACHLOROMETHANE	340
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Formula Index of Systems

=====			
C6H12	1-HEXENE		
C2CL4	TETRACHLOROETHYLENE		341
C2HCL3	TRICHLOROETHYLENE		342
C2H2CL4	1,1,2,2-TETRACHLOROETHANE		343
C2H3CL3	1,1,1-TRICHLOROETHANE		344
C2H3CL3	1,1,2-TRICHLOROETHANE		345
C3H5CL3	1,2,3-TRICHLOROPROPANE		346
	C6H14	HEXANE	651
C3H7BR	PROPYL BROMIDE		347
C4H11N	BUTYLAMINE		348
C4H11N	DIETHYLAMINE		349
C6H6	BENZENE		350
C6H14	HEXANE		351-353 353 R
C6H15N	DIISOPROPYLAMINE		354
C6H15N	DIPROPYLAMINE		355
C6H15N	HEXYLAMINE		356
C6H15N	TRIETHYLAMINE		357
C7H8	TOLUENE		358-360
=====			
C6H12	METHYLCYCLOPENTANE		
CCL4	TETRACHLOROMETHANE		361
C3H8S	1-PROPANETHIOL		362
C6H6	BENZENE		363-368 368 R
	C6H14	HEXANE	652-658
C6H14	HEXANE		369-374
C7H8	TOLUENE		375
=====			
C6H12	2-METHYL-1-PENTENE		
C6H6	BENZENE		376-377
=====			
C6H12	4-METHYL-1-PENTENE		
C6H6	BENZENE		378-380
=====			
C6H14	2,2-DIMETHYLBUTANE		
CCL4	TETRACHLOROMETHANE		381
C6H6	BENZENE		382-384
C6H14	HEXANE		385
C16H34	HEXADECANE		386
=====			
C6H14	2,3-DIMETHYLBUTANE		
CCL4	TETRACHLOROMETHANE		387

Formula Index of Systems

C6H14		2,3-DIMETHYLBUTANE
CHCL3	CHLOROFORM	388-390 390 R
C6H6	BENZENE	391-393
C6H14	HEXANE	394
C7H14	CYCLOHEPTANE	395
C8H16	CYCLOOCTANE	396
C16H34	HEXADECANE	397

C6H14		HEXANE
CCL4	TETRACHLOROMETHANE	398-403
CD3I	TRIDEUTEROIODIDE	404-409
CD5N	PERDEUTEROMETHYLAMINE	410-419
CHBR3	TRIBROMOMETHANE	420-422
CHCL3	CHLOROFORM	423-432 432 R
CH2D3N	TRIDEUTEROMETHYLAMINE	433-437
CH3D2N	N,N-DEUTEROMETHYLAMINE	438-442
CH5N	METHYLAMINE	443-452
C2CL4	TETRACHLOROETHYLENE	453
C2D7N	PERDEUTERODIMETHYLAMINE	454-461
C2HCL3	TRICHLOROETHYLENE	462-463
C2HD6N	HEXADEUTERODIMETHYLAMINE	464-471
C2H2CL4	1,1,2,2-TETRACHLOROETHANE	472
C2H3CL3	1,1,1-TRICHLOROETHANE	473
C2H3CL3	1,1,2-TRICHLOROETHANE	474
C2H5D2N	N,N-DEUTEROETHYLAMINE	475-478
C2H5I	ETHYL IODIDE	479-480
C2H5NO2	NITROETHANE	481-483 483 R
C2H6DN	N-DEUTERODIMETHYLAMINE	484-490
C2H7N	DIMETHYLAMINE	491-503
C2H7N	ETHYLAMINE	504-507
C3H5CL3	1,2,3-TRICHLOROPROPANE	508
C3H7NO2	1-NITROPROPANE	509
C3H7NO2	2-NITROPROPANE	510
C3H8S	1-PROPANETHIOL	511
C3H9N	PROPYLAMINE	512-514
C3H9N	TRIMETHYLAMINE	515-517
C4H11N	BUTYLAMINE	518
C4H11N	DIETHYLAMINE	519
C6F6	HEXAFLUOROBENZENE	520-521

Formula Index of Systems

=====			
C6H14	HEXANE		
C6F14	PERFLUOROHXANE	522-525 525 R	
C6H3CL3	1,2,4-TRICHLOROBENZENE	526-527	
C6H5CL	CHLOROBENZENE	528-530	
	C6H6	BENZENE	659-661
C6H5NO2	NITROBENZENE	531-533	
C6H6	BENZENE	534-559 559 R	
	C7H8	TOLUENE	662-663
	C8H10	P-XYLENE	664-665
C6H7N	ANILINE	560-580	
C6H12	METHYLCYCLOPENTANE	581	
C6H14	2-METHYLPENTANE	582	
C6H14	3-METHYLPENTANE	583	
C6H15N	DIISOPROPYLAMINE	584	
C6H15N	DIPROPYLAMINE	585	
C6H15N	HEXYLAMINE	586-589	
C6H15N	TRIETHYLAMINE	590	
C7H8	TOLUENE	591-595	
C7H14	METHYLCYCLOHEXANE	596-597	
C7H16	HEPTANE	598-606	
C8H10	P-XYLENE	607-608	
C8H18	OCTANE	609-613	
C16H34	HEXADECANE	614-618	
=====			
C6H14	2-METHYLPENTANE		
CCL4	TETRACHLOROMETHANE	619	
C2H5NO2	NITROETHANE	620	
C3H8S	1-PROPANETHIOL	621	
C6H6	BENZENE	622-624	
C16H34	HEXADECANE	625	
=====			
C6H14	3-METHYLPENTANE		
CCL4	TETRACHLOROMETHANE	626	
C7H8	TOLUENE	627-629	
C16H34	HEXADECANE	630	
=====			



Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE	
1,3-PLTADIENE		C4H6		
	BENZENE	C6H6	14	
	BUTANE	C4H10	11-13	
	1-BUTENE	C4H8	8-10 10 R	
	CARBON DISULFIDE	CS2	6	
	2-CHLORO-1,3-BUTADIENE	C4H5CL	7	
	DICHLOROMETHANE	CH2CL2	4	
	NITROMETHANE	CH3NO2	5	
	STYRENE	C8H8	15-16	
	TETRACHLOROMETHANE	CCL4	3	
BUTANE		C4H10		
	N-DEUTEROETHYLAMINE	C2H5D2N	23-27	
	ETHYLAMINE	C2H7N	28	
	ETHYL CHLORIDE	C2H5CL	22	
	HEXANE	C6H14	31-35	
	METHYLAMINE	CH5N	19-21	
	PENTANE	C5H12	30	
	PERFLUOROCYCLOBUTANE	C4F8	29	
1-BUTENE		C4H8		
	BUTANE	C4H10	17	
CYCLOHEXANE		C6H12		
	ANILINE	C6H7N	242-257 257 R	
	BENZENE	C6H6	204-241 240-241 R	
		ANILINE	C6H7N	639
		HEXANE	C6H14	640-647
		TOLUENE	C7H8	648
	BROMOBENZENE	C6H5BR	196-201	
	CARBON DISULFIDE	CS2	153-154	
	CHLOROBENZENE	C6H5CL	202	
	CHLOROCYCLOHEXANE	C6H11CL	258-261	
	CHLORODIFLUOROMETHANE	CHCLF2	151-152	
	CYCLOHEXYLAMINE	C6H13N	263-269	
	1,2-DIBROMOETHANE	C2H4BR2	157	

Alphabetical Index of Systems

CYCLOHEXANE

	C6H12		
1,2-DICHLOROETHANE	C2H4CL2	158-163	R
		163	
DIMETHYLBUTANE	C6H14	272	
DODECANE	C12H26	330-333	
EICOSANE	C20H42	337-339	
ETHYLBENZENE	C8H10	308-310	
HEPTANE	C7H16	300-306	R
		306	
HEXADECANE	C16H34	334-336	
HEXAFLUOROBENZENE	C6F6	186-191	R
		191	
HEXAMETHYLENIMINE	C6H13N	270-271	
HEXANE	C6H14	273-277	R
		277	
METHYLANILINE	C7H9N	292-294	
METHYLCYCLOHEXANE	C7H14	295	
N-METHYLCYCLOHEXYLAMINE	C7H15N	296-299	R
		299	
METHYLCYCLOPENTANE	C6H12	262	
N-METHYL FORMAMIDE	C2H5NO	164-165	
NITROBENZENE	C6H5NO2	203	
NITROMETHANE	CH3NO2	BENZENE	C6H6 636
OCTANE	C8H18	320-323	
1-OCTENE	C8H16	319	
PENTACHLOROETHANE	C2HCL5	156	
PERFLUOROCYCLOHEXANE	C6F12	192-195	
PIPERIDINE	C5H11N	183-185	R
		185	
PYRIDINE	C5H5N	171-182	
PYRROLIDINE	C4H9N	168-170	R
		170	
TETRACHLOROMETHANE	CCl4	139-150	R
		150	
THIAZOLE	C3H3NS	166	
THIOPHENE	C4H4S	167	
TOLUENE	C7H8	278-291	
		HEPTANE	C7H16 649-650
TRICHLOROETHYLENE	C2HCL3	155	
		BENZENE	C6H6 637-638
TRIMETHYLBUTANE	C7H16	307	
2,2,4-TRIMETHYLPENTANE	C8H18	324-329	R
		329	
M-XYLENE	C8H10	313-314	
O-XYLENE	C8H10	311-312	
P-XYLENE	C8H10	315-318	

Alphabetical Index of Systems

=====			
CYCLOHEXENE	C6H10		
BENZENE	C6H6		130-136 136 R
CYCLOHEXANE	C6H12		157-138
1,2-DICHLOROETHANE	C2H4CL2		129
		CYCLOHEXANE	C6H12 634-635
TETRACHLOROMETHANE	CCL4		128
=====			
CYCLOPENTADIENE	C5H6		
ISOPRENE	C5H8		36
		2-METHYL-2-BUTENE	C5H10 631
2-METHYL-2-BUTENE	C5H10		37
=====			
CYCLOPENTANE	C5H10		
BENZENE	C6H6		69- 73
CARBON DISULFIDE	CS2		63- 66 66 R
CHLOROFORM	CHCL3		62
CIS-DECAHYDRONAPHTHALENE	C10H18		75
TRANS-DECAHYDRONAPHTHALENE	C10H18		76
2,3-DIMETHYLBUTANE	C6H14		74
2-PROPANETHIOL	C3H8S		68
TETRACHLOROETHYLENE	C2CL4		67
TETRACHLOROMETHANE	CCL4		60- 61
=====			
2,2-DIMETHYLBUTANE	C6H14		
BENZENE	C6H6		382-384
HEXADECANE	C16H34		386
HEXANE	C6H14		385
TETRACHLOROMETHANE	CCL4		381
=====			
2,3-DIETHYLBUTANE	C6H14		
BENZENE	C6H6		391-393
CHLOROFORM	CHCL3		388-390 390 R
CYCLOHEPTANE	C7H14		395
CYCLOOCTANE	C8H16		396
HEXADECANE	C16H34		397
HEXANE	C6H14		394
TETRACHLOROMETHANE	CCL4		387
=====			
HEXANE	C6H14		
ANILINE	C6H7N		560-580

Alphabetical Index of Systems

HEXANE

C6H14		
BENZENE	C6H6	534-559 559 R
	TOLUENE	C7H8 662-663
	P-XYLENE	C8H10 664-665
BUTYLAMINE	C4H11N	518
CHLOROBENZENE	C6H5CL	528-530
	BENZENE	C6H6 659-661
CHLOROFORM	CHCL3	423-432 432 R
N-DEUTERODIMETHYLAMINE	C2H6DN	484-490
N,N-DEUTEROETHYLAMINE	C2H5D2N	475-478
N,N-DEUTEROMETHYLAMINE	CH3D2N	438-442
DIETHYLAMINE	C4H11N	519
DIISOPROPYLAMINE	C6H15N	584
DIMETHYLAMINE	C2H7N	491-503
DIPROPYLAMINE	C6H15N	585
ETHYLAMINE	C2H7N	504-507
ETHYL IODIDE	C2H5I	479-480
HEPTANE	C7H16	598-606
HEXADECANE	C16H34	614-618
HEXADEUTERODIMETHYL- AMINE	C2HD6N	464-471
HEXAFLUOROBENZENE	C6F6	520-521
HEXYLAMINE	C6H15N	586-589
METHYLAMINE	CH5N	443-452
METHYLCYCLOHEXANE	C7H14	596-597
METHYLCYCLOPENTANE	C6H12	581
2-METHYLPENTANE	C6H14	582
3-METHYLPENTANE	C6H14	583
NITROBENZENE	C6H5NO2	531-533
NITROETHANE	C2H5NO2	481-483 483 R
1-NITROPROPANE	C3H7NO2	509
2-NITROPROPANE	C3H7NO2	510
OCTANE	C8H18	609-613
PERDEUTERODIMETHYL- AMINE	C2D7N	454-461
PERDEUTEROMETHYLAMINE	CD5N	410-419
PERFLUOROHEXANE	C6F14	522-525 525 R
1-PROPANETHIOL	C3H8S	511
PROPYLAMINE	C3H9N	512-514
1,1,2,2-TETRACHLOROETHANE	C2H2CL4	472
TETRACHLOROETHYLENE	C2CL4	453

Alphabetical Index of Systems

=====			
HEXANE	C6H14		
	TETRACHLOROMETHANE	CCL4	398-403
	TOLUENE	C7H8	591-595
	TRIBROMOMETHANE	CHBR3	420-422
	1,2,4-TRICHLOROENZENE	C6H3CL3	526-527
	1,1,1-TRICHLOROETHANE	C2H3CL3	473
	1,1,2-TRICHLOROETHANE	C2H3CL3	474
	TRICHLOROETHYLENE	C2HCL3	462-463
	1,2,3-TRICHLOROPROPANE	C3H5CL3	508
	TRIDEUTEROIODIDE	CD3I	406-409
	TRIDEUTEROMETHYLAMINE	CH2D3N	433-437
	TRIETHYLAMINE	C6H15N	590
	TRIMETHYLAMINE	C3H9N	515-517
	P-XYLENE	C8H10	607-608
=====			
1-HEXENE	C6H12		
	BENZENE	C6H6	350
	BUTYLAMINE	C4H11N	348
	DIETHYLAMINE	C4H11N	349
	DIISOPROPYLAMINE	C6H15N	354
	DIPROPYLAMINE	C6H15N	355
	HEXANE	C6H14	351-353 353 R
	HEXYLAMINE	C6H15N	356
	PROPYL BROMIDE	C3H7BR	347
	1,1,2,2-TETRACHLOROETHANE	C2H2CL4	343
	TETRACHLOROETHYLENE	C2CL4	341
	TETRACHLOROMETHANE	CCL4	340
	TOLUENE	C7H8	358-360
	1,1,1-TRICHLOROETHANE	C2H3CL3	344
	1,1,2-TRICHLOROETHANE	C2H3CL3	345
	TRICHLOROETHYLENE	C2HCL3	342
	1,2,3-TRICHLOROPROPANE	C3H5CL3	346
		HEXANE	C6H14 651
	TRIETHYLAMINE	C6H15N	357
=====			
ISOBUTENE	C4H8		
	ISOPRENE	C5H8	18
=====			
ISOPPENE	C5H8		
	ACETONITRILE	C2H3N	39-40
		2-METHYL-2-BUTENE	C5H10 632-633
=====			

Alphabetical Index of Systems

=====		
ISOPRENE	C5H8	

N,N-DIMETHYLFORMAMIDE	C3H7NO	44
DIMETHYLSULFOXIDE	C2H6OS	41- 43
2-METHYLBUTANE	C5H12	56
2-METHYL-1-BUTENE	C5H10	46- 47
2-METHYL-2-BUTENE	C5H10	48- 53
3-METHYL-1-BUTENE	C5H10	54- 55
NITROMETHANE	CH3NO2	38
TR-1,3-PENTADIENE	C5H8	45
=====		
2-METHYLBUTANE	C5H12	

ACETONITRILE	C2H3N	88
CARBON DISULFIDE	CS2	86-87
N,N-DIMETHYLFORMAMIDE	C3H7NO	89
=====		
2-METHYL-1-BUTENE	C5H10	

2-METHYL-2-BUTENE	C5H10	78
NITROMETHANE	CH3NO2	77
=====		
2-METHYL-2-BUTENE	C5H10	

ACETONITRILE	C2H3N	80- 82
N,N-DIMETHYLFORMAMIDE	C3H7NO	83
2-METHYLBUTANE	C5H12	84
NITROMETHANE	CH3NO2	79
=====		
METHYLCYCLOPENTANE	C6H12	

BENZENE	C6H6	363-368 368 R
	HEXANE	C6H14
		652-658
HEXANE	C6H14	369-374
1-PROPANETHIOL	C3H8S	362
TETRACHLOROMETHANE	CCL4	361
TOLUENE	C7H8	375
=====		
2-METHYLPENTANE	C6H14	

BENZENE	C6H6	622-624
HEXADECANE	C16H34	625
NITROETHANE	C2H5NO2	620
1-PROPANETHIOL	C3H8S	621
TETRACHLOROMETHANE	CCL4	619

Alphabetical Index of Systems

3-METHYLPENTANE	C6H14	
HEXADECANE	C16H34	630
TETRACHLOROMETHANE	CCL4	626
TOLUENE	C7H8	627-629
2-METHYL-1-PENTENE	C6H12	
BENZENE	C6H6	376-377
4-METHYL-1-PENTENE	C6H12	
BENZENE	C6H6	378-380
NEOPENTANE	C5H12	
PENTANE	C5H12	95-99
TETRAMETHYLSILANE	C4H12SI	90-94
TR-1,3-PENTADIENE	C5H8	
DIMETHYLSULFOXIDE	C2H6OS	57-59
PENTANE	C5H12	
ACETONITRILE	C2H3N	101-102
ACRYLONITRILE	C3H3N	103-104
BENZENE	C6H6	114-118
CYCLOHEXANE	C6H12	119
DICHLOROMETHANE	CH2CL2	100
HEPTANE	C7H16	126-127
HEXANE	C6H14	122-123
METHYLCYCLOHEXANE	C7H14	124-125
METHYLCYCLOPENTANE	C6H12	120-121
PENTYL BROMIDE	C5H11BR	106-113
1-PROPANETHIOL	C3H8S	105
1-PENTENE	C5H10	
ACETONITRILE	C2H3N	85
VINYLAETHYLENE	C4H4	
BENZENE	C6H6	1
P-XYLENE	CRH10	2