

**J. Gmehling
U. Onken
W. Arlt**

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

Aliphatic Hydrocarbons

C₇ – C₁₈



Chemistry Data Series

Vol. I, Part 6b

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Vapor-Liquid Equilibrium Data Collection

6b

Aliphatic Hydrocarbons

C₇ – C₁₈

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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6b

Aliphatic Hydrocarbons

C₇—C₁₈

Systems with:

1,5-Cyclooctadiene	Methylcyclohexane
Decahydronaphthalene	3-Methylheptane
Decane	3-Methylhexane
α -Dicyclopentadiene	Nonane
2,3-Dimethylpentane	1-Octadecene
2,4-Dimethylpentane	Octane
Dodecane	1-Octene
Ethylcyclohexane	α -Pinene
Heptadecane	Tetradecane
Heptane	2,2,3-Trimethylbutane
1-Heptene	1,3,5-Trimethylcyclohexane
2-Heptene	2,2,5-Trimethylhexane
3-Heptene	2,2,4-Trimethylpentane
Hexadecane	Undecane
1-Hexadecene	2-Vinyl-(2,2,1)-bicycloheptane
Isopropylcyclohexane	2-Vinyl-(2,2,1)-bicyclo-5-heptene

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Alcohols	2a (1977)
Alcohols and Phenols	2b (1978)
Supplement 1	2c (1982)
Supplement 2	2d (1982)
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Aldehydes, Ketones, Ethers	3/4 (1979)
Supplement 1, Aldehydes	3a (1993)
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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

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

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Octane	231
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Nonane	348
2,2,5-Trimethylhexane	357

α -Dicyclopentadiene	359
α -Pinene	361
trans-Decahydronaphthalene	372
Decane	383
Undecane	409
Dodecane	410
Tetradecane	425
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Heptadecane	453
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Formula Index of Systems

R=RECOMMENDED VALUES

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	4TH COMPONENT	PAGE
C7H14	1-HEPTENE			
C4H9Br	BUTYL BROMIDE			1
C7H16	HEPTANE			2
		C3H18	OCTANE	463
C8H18	OCTANE			3
C7H14	2-HEPTENE			
C5H7N	ANILINE			4
C7H14	3-HEPTENE			
C7H16	HEPTANE			5
C7H14	METHYLCYCLOHEXANE			
CCL4	TETRACHLOROMETHANE			6
C2H5NO2	NITROETHANE			7
C5F6	HEXAFLUOROBENZENE			8- 9
C5H6	BENZENE			10- 12
C5H7N	ANILINE			13- 18
		C7H8	TOLUENE	18 R 464-466
C5H11Cl	CHLOROCYCLOHEXANE			19- 21
C5H13N	CYCLOHEXYLAMINE			22- 25
C7F14	PERFLUOROMETHYLCYCLOHEXANE			26- 29
C7H8	TOLUENE			30- 46
		C7H16	HEPTANE	46 R 467-468
C7H16	HEPTANE			47- 53
				53 R
C8H10	ETHYLBENZENE			54- 56
C3H13	2,2,4-TRIMETHYLPENTANE			57- 59
C7H16	2,3-DIMETHYLPENTANE			
C6H6	BENZENE			60
		C12F27N	PERFLUOROTRIBUTYLAMINE	469
C7H16	2,4-DIMETHYLPENTANE			
CCL4	TETRACHLOROMETHANE			61
C5H6	BENZENE			62- 66
				66 R
C7H16	HEPTANE			
CCL4	TETRACHLOROMETHANE			67- 73

Formula Index of Systemes

=====			
C7H15	HEPTANE		
C7H5Cl3	CHLOROFORM		74-78 78 R
		C6H6	BENZENE
			470
C7H3N	ACETONITRILE		70-85
		C6H6	BENZENE
			471-474
C2H5Br	ETHYL BROMIDE		86
C2H5I	ETHYL IODIDE		87-89 R
C2H5NO	N-METHYLFORMAMIDE		90-91
C2H5NO2	NITROETHANE		92
C3H7NO	N,N-DIMETHYLFORMAMIDE		93-98
C3H7NO2	1-NITROPROPANE		99
C3H7NO2	2-NITROPROPANE		100
C4Cl3F7	2,2,3-TRICHLOROHEPTAFLUOROBUTANE		101
C4H4S	THIOPHENE		102
		C6H6	BENZENE
			475
C4H9Br	BUTYL BROMIDE		103
C4H9Cl	BUTYL CHLORIDE		104
C4H9NO	METHYL ETHYL KETOXIME		105-108 108 R
C4H11N	BUTYLAMINE		109-110
C4H11N	DIETHYLAMINE		111-112
C5H5N	PYRIDINE		113-116
C5H5Cl	CHLOROBENZENE		117-119
C6H6	BENZENE		120-158 158 R
C6H7N	ANILINE		159-161
		C7H8	TOLUENE
			476
C6H15N	TRIETHYLAMINE		162-164 164 R
C7F15	PERFLUOROHEPTANE		165-167
C7H8	TOLUENE		168-185 185 R
C8H10	P-XYLENE		186-187
C8H18	OCTANE		188-195
C8H18	2,2,4-TRIMETHYLPENTANE		196-197
C9H12	ISOPROPYLBENZENE		198-200
=====			
C7H15	3-METHYLHEXANE		
C5H6	BENZENE		201-202
C9H12	PROPYLBENZENE		203-205
=====			
C7H16	2,2,3-TRIMETHYLBUTANE		
C5H5	BENZENE		206-207

Formula Index of Systemes

=====				
C3H12	1,5-CYCLOOCTADIENE			
C9H12	4,7,8,9-TETRAHYDROINDENE		209-209	
C9H12	2-VINYLCYCLO-5-HEPTENE		210-211	
C10H12	ALPHA-DICYCLOPENTADIENE (ENDO)		212-213	
=====				
C3H14	ETHYLCYCLOHEXANE			
C3H10	ETHYLBENZENE		214	
C3H13	OCTANE		215	
=====				
C3H15	1-OCTENE			
CCL4	TETRACHLOROMETHANE		216	
C5H6	BENZENE		217-218	
C3H10	ETHYLBENZENE		219	
C3H13	OCTANE		220-223	
=====				
C3H18	3-METHYLHEPTANE			
CCL4	TETRACHLOROMETHANE		224-226	
C7F16	PERFLUOROHEPTANE		227-230	
=====				
C3H18	OCTANE			
CCL4	TETRACHLOROMETHANE		231-234	
C2H5NO2	NITROETHANE		235	
		C8H18	2,2,4-TRIMETHYLPENTANE	477
C4H7N	BUTYRONITRILE		236	
C5H5N	PYRIDINE		237-240 240 R	
C6H5NO2	NITROBENZENE		241	
C5H6	BENZENE		242-250	
C5H12	CYCLOHEXANE		251-253	
C7H8	TOLUENE		254-269 269 R	
		C8H10	ETHYLBENZENE	478
C3H10	ETHYLBENZENE		270-274 274 R	
C3H10	P-XYLENE		275	
C8H16	ETHYLCYCLOHEXANE		276-281 281 R	
C8H18	2,2,4-TRIMETHYLPENTANE		282-283	
=====				
C3H19	2,2,4-TRIMETHYLPENTANE			
CCL4	TETRACHLOROMETHANE		284-290 290 R	
=====				

Formula Index of Systemes

C8H18	2,2,4-TRIMETHYLPENTANE	
C8Br3	TRIBROMOMETHANE	291
C8H5NO2	NITROETHANE	292-295 295 R
C8H7N	BUTYRONITRILE	296
C5H5N	PYRIDINE	297-301
C6H5NO2	NITROBENZENE	302
C6H6	BENZENE	303-312 312 R
C6H7N	ANILINE	313-318
C7F16	PERFLUOROHEPTANE	319-321
C7H8	TOLUENE	322-330 330 R
C8H10	ETHYLBENZENE	331-333
C9H12	2-VINYL-(2,2,1)-BICYCLO-5-HEPTENE	
C9H12	2-ETHYLIDENE-(2,2,1)-BICYCLO-5-HEPTENE	334-335
C9H12	4,7,8,9-TETRAHYDROINDENE	336
C9H14	2-VINYL-(2,2,1)-BICYCLOHEPTANE	337-338
C9H16	2-ETHYL-(2,2,1)-BICYCLOHEPTANE	339-340
C9H14	2-VINYL-(2,2,1)-BICYCLOHEPTANE	
C9H16	2-ETHYL-(2,2,1)-BICYCLOHEPTANE	341-342
C9H18	ISOPROPYLCYCLOHEXANE	
C6F6	HEXAFLUOROBENZENE	343
C9H18	CIS-(1,3,5)-TRIMETHYLCYCLOHEXANE	
C6F12	PERFLUOROCYCLOHEXANE	344-347
C9H20	NONANE	
C8H9	METHYLAMINE	348-351
C5H5N	PYRIDINE	352-355 355 R
C7H9N	2,4-DIMETHYLPYRIDINE	356
C9H20	2,2,5-TRIMETHYLHEXANE	
CCl4	TETRACHLOROMETHANE	357
C8H10	ETHYLBENZENE	358
C10H12	ALPHA-DICYCLOPENTADIENE	
C6H6	BENZENE	359
C7H8	TOLUENE	360

Formula Index of Systemes

=====				
C10H16	ALPHA-PINENE			
C10H16	DELTA-3-CARENE		361	
C10H16	LIMONENE		362	
C10H16	BETA-PINENE		363-371	
=====				
C10H18	TRANS-DECAHYDRONAPHTHALENE			
C9H12	1,2,3-TRIMETHYLBENZENE		372-373	
C9H12	1,2,4-TRIMETHYLBENZENE		374-375	
C10H22	DECANE		376-382	
=====				
C10H22	DECANE			
CH4S	METHANETHIOL		383	
C5H5N	PYRIDINE		384-386	
C6H5CL	CHLOROBENZENE		387-392	
C7H9N	2,6-DIMETHYLPYRIDINE		393	
C7H9N	O-METHYLANILINE		394	
C9H12	1,2,3-TRIMETHYLBENZENE		395-399	
		C9H12	1,2,4-TRIMETHYLBENZENE	479-480
		C9H12	1,2,4-TRIMETHYLBENZENE	
		C9H12	1,3,5-TRIMETHYLBENZENE	485-486
		C9H12	1,2,5-TRIMETHYLBENZENE	481
		C9H12	1,3,5-TRIMETHYLBENZENE	482
C9H12	1,2,4-TRIMETHYLBENZENE		480-484	
		C9H12	1,2,5-TRIMETHYLBENZENE	483-484
C9H12	1,3,5-TRIMETHYLBENZENE		485-488	
=====				
C11H24	UNDECANE			
C7H9N	2,4-DIMETHYLPYRIDINE		409	
=====				
C12H26	DODECANE			
C10H8	NAPHTHALENE		410-411	
C15H32	1-HEXADECENE		412-417	
C18H36	1-OCTADECENE		418-424	
=====				
C14H30	TETRADECANE			
C6H6	BENZENE		425-427	
C10H8	NAPHTHALENE		428-435	
C15H32	1-HEXADECENE		436-444	
=====				
C16H32	1-HEXADECENE			
C10H8	NAPHTHALENE		445	
=====				

Formula Index of Systemes

=====		
C16H34	HEXADECANE	

CCL4	TETRACHLOROMETHANE	446-447

C5H6	BENZENE	448-452
=====		
C17H36	HEPTADECANE	

C5H6	BENZENE	453-455
=====		
C18H36	1-OCTADECENE	

C10H8	NAPHTHALENE	456-462

Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE
1,5-CYCLOOCTADIENE		C8H12	
	ALPHA-DICYCLOPENTADIENE (ENDO)	C10H12	212-213
	4,7,3,9-TETRAHYDROINDENE	C9H12	208-209
	2-VINYL-(2,2,1)- BICYCLO-5-HEPTENE	C9H12	210-211
TRANS-DECAHYDRONAPHTHALENE		C10H18	
	DECANE	C10H22	376-382
	1,2,3-TRIMETHYLBENZENE	C9H12	372-373
	1,2,4-TRIMETHYLBENZENE	C9H12	374-375
DECANE		C10H22	
	CHLOROBENZENE	C6H5Cl	387-392
	2,6-DIMETHYLPYRIDINE	C7H9N	393
	METHANETHIOL	CH4S	383
	O-METHYLANILINE	C7H9N	394
	PYRIDINE	C5H5N	384-386
	1,2,3-TRIMETHYLBENZENE	C9H12	395-399
		1,2,4-TRIMETHYLBENZENE	C9H12 479-480
		1,2,4-TRIMETHYLBENZENE	C9H12
		1,3,5-TRIMETHYLBENZENE	C9H12 485-486
		1,2,5-TRIMETHYLBENZENE	C9H12 481
		1,3,5-TRIMETHYLBENZENE	C9H12 482
	1,2,4-TRIMETHYLBENZENE	C9H12	400-404
		1,2,5-TRIMETHYLBENZENE	C9H12 483-484
	1,3,5-TRIMETHYLBENZENE	C9H12	405-408
ALPHA-DICYCLOPENTADIENE		C10H12	
	BENZENE	C6H6	359
	TOLUENE	C7H8	360
2,3-DIETHYLPENTANE		C7H16	
	BENZENE	C6H6	60
		PERFLUOROTRIBUTYL- AMINE	C12F27N 469
2,4-DIMETHYLPENTANE		C7H16	
	BENZENE	C6H6	62-66 R
	TETRACHLOROMETHANE	CCl4	61

Alphabetical Index of Systems

DDDECANE	C12H26			
1-HEXADECENE	C16H32		412-417	
NAPHTHALENE	C10H8		419-411	
1-OCTADECENE	C18H36		418-424	
ETHYLCYCLOHEXANE	C8H16			
ETHYLBENZENE	C8H10		214	
OCTANE	C8H18		215	
HEPTADECANE	C17H36			
BENZENE	C6H6		453-455	
HEPTANE	C7H16			
ACETONITRILE	C2H3N		79- 85	
		BENZENE	C6H6	471-474
ANILINE	C6H7N		159-161	
		TOLUENE	C7H8	476
BENZENE	C6H6		120-158 158 R	
BUTYLAMINE	C4H11N		109-110	
BUTYL BROMIDE	C4H9BR		103	
BUTYL CHLORIDE	C4H9CL		104	
CHLOROBENZENE	C6H5CL		117-119	
CHLOROFORM	CHCL3		74- 78 78 R	
		BENZENE	C6H6	470
DIETHYLAMINE	C4H11N		111-112	
N,N-DIMETHYLFORMAMIDE	C3H7NO		93- 98	
ETHYL BROMIDE	C2H5BR		86	
ETHYL IODIDE	C2H5I		87- 89 R	
ISOPROPYLBENZENE	C9H12		198-200	
METHYL ETHYL KETOXIME	C4H9NO		105-108 108 R	
N-METHYLFORMAMIDE	C2H5NO		99- 91	
NITROETHANE	C2H5NO2		92	
1-NITROPROPANE	C3H7NO2		90	
2-NITROPROPANE	C3H7NO2		100	
OCTANE	C8H18		188-195	
PERFLUOROHEPTANE	C7F16		165-167	
PYRIDINE	C5H5N		113-116	
TETRACHLOROMETHANE	CCl4		67- 73	
THIOPHENE	C4H4S		102	
		BENZENE	C6H6	475

Alphabetical Index of Systems

=====			
HEPTANE	C7H16		
	TOLUENE	C7H8	163-185 185 R
	2,2,3-TRICHLOROHEPTAFLUORO- BUTANE	C4CL3F7	101
	TRIETHYLAMINE	C6H15N	162-164 164 R
	2,2,4-TRIMETHYLPENTANE	C8H18	196-197
	P-XYLENE	C8H10	186-187
=====			
1-HEPTENE	C7H14		
	BUTYL BROMIDE	C4H9BR	1
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