

**J. Gmehling
U. Onken
P. Grenzheuser**

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

Carboxylic Acids, Anhydrides, Esters



Chemistry Data Series

Vol. I, Part 5

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Vapor-Liquid Equilibrium Data Collection

5

Carboxylic Acids, Anhydrides, Esters

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

J. Gmehling, U. Onken, P. Grenzheuser

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5

Carboxylic Acids, Anhydrides, Esters**Systems with:****Carboxylic Acids:**

Acetic acid	Methacrylic acid
Acrylic acid	Myristic acid
Benzoic acid	Octanoic acid
Butyric acid	Oleic acid
Chloroacetic acid	Palmitic acid
Decanoic acid	Propionic acid
Formic acid	Stearic acid
Hexanoic acid	Trifluoroacetic acid
Isobutyric acid	Valeric acid
Lauric acid	

Anhydrides:

Acetic anhydride	Maleic anhydride
------------------	------------------

Esters:

Allyl acetate	Methyl benzoate
Benzyl acetate	Methyl borate
2,3-Butanediol diacetate	Methyl decanoate
Butyl acetate	Methylene diacetate
Butyl formate	Methyl formate
Butyl methacrylate	Methyl hexanoate
Cyclohexyl acetate	Methyl laurate
Diethyl oxalate	Methyl-9,12-linoleate
Dimethyl carbonate	Methyl methacrylate
Dimethyl isophthalate	Methyl myristate
Ethyl acetate	Methyl octanoate
Ethyl acetoacetate	Methyl palmitate
Ethyl acrylate	Methyl propionate
Ethyl butyrate	Methyl salicylate
Ethyl formate	Methyl stearate
Heptyl acetate	Methyl m-toluate
Isobutyl acetate	Octyl acetate
Isopentyl acetate	Pentyl acetate
Isopentyl formate	Propyl acetate
Isopropenyl acetate	Propylene carbonate
Isopropyl acetate	Propyl formate
Isopropyl formate	Triethyl orthoacetate
Methyl acetate	Triethyl orthoformate
Methyl acrylate	Vinyl acetate

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

AUTHORS' PREFACE

As we explained in the preface to part 6, this part 5 had to be postponed, because we intended to include the effect of dimerization on vapor phase non-ideality also for systems with more than one associating component, i.e. carboxylic acids. This work has now been completed by Peter Grenzheuser, who is therefore co-author of this part. He worked out the calculation procedures for the correlation of data from binary systems consisting of two carboxylic acids and from ternary systems containing up to three carboxylic acids, and for the optimization of parameters of these systems. Besides, he incorporated vapor phase dimerization into the two consistency tests, in order to be able to use them with binary systems containing carboxylic acids.

Again, many colleagues have helped us by sending us preprints and research reports with VLE data. We take this opportunity to thank all of them, especially Prof. Dr. K. Quitzsch (Karl-Marx-University, Leipzig), Prof. F. Aguirre Ode (University of Santa Maria, Valparaiso) and Dr. D. Zudkevitch (Allied Chemical Corporation). Likewise we should like to mention with gratitude the continuous endeavour of Dr. R. Eckermann and Dipl.-Ing. C. Hammer from DECHEMA (Frankfurt/Main) and their efforts in editing the data series.

From our team at Dortmund the following members have contributed to this part: Mrs. A. Brunk, Dipl.-Ing. B. Kolbe, Mrs. L. Kunzner, Dipl.-Chem. J. Menke, Mrs. G. Obermann, Dipl.-Chem. U. Schwaitzer, Dipl.-Chem. U. Weidlich. We should also like to repeat our thanks to Mr. T. Blaszyk from the computer center of the University of Dortmund.

Dortmund, September 1982

Ulfert Onken Jürgen Gmehling Peter Grenzheuser

PREFACE OF EDITORS

Subjects of the Dechema Chemistry Data 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 research work of Dr. Gmehling, Prof. Onken and Dipl.-Chem. Arit 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, September 1982

Dieter Behrens
Reiner Eckermann

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Ethyl butyrate	594
Isobutyl acetate	596
Methyl hexanoate	598
Pentyl acetate	603
Triethyl orthoformate	606
Methyl benzoate	618
Methyl salicylate	621
Butyl methacrylate	623
Triethyl orthoacetate	624
Benzyl acetate	635

Methyl m-toluate	638
Heptyl acetate	639
Methyl octanoate	640
Octyl acetate	644
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Formula Index of Systems

R = RECOMMENDED VALUES

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CH2O2	FORMIC ACID		
CHCL3	CHLOROFORM		1
		C2H4O2 ACETIC ACID	273-274
C2H4CL2	1,2-DICHLOROETHANE		2- 6
C2H4O2	ACETIC ACID		7- 12
		C3H6O2 PROPIONIC ACID	275-277
C3H4O2	ACRYLIC ACID		13
C3H6O2	PROPIONIC ACID		14- 16
C3H7CL	1-CHLOROPROPANE		17
C3H7CL	ISOPROPYL CHLORIDE		18
C3H7NO	N,N-DIMETHYLFORMAMIDE		19- 27 27 R
C4H8O2	BUTYRIC ACID		28
C4H8O2	ISOPROPYL FORMATE		29
C4H8O2	PROPYL FORMATE		30
C4H9CL	BUTYL CHLORIDE		31
C4H9CL	TERT-BUTYL CHLORIDE		32
C4H9CL	ISOBUTYL CHLORIDE		33
C5H10O2	BUTYL FORMATE		34- 36
C5H10O2	VALERIC ACID		37- 39
C6H6	BENZENE		40- 42
C6H12O2	ISOPENTYL FORMATE		43
C6H15N	TRIETHYLAMINE		44- 47
C7H8	TOLUENE		48
C8H10	P-XYLENE		49
C2HF3O2	TRIFLUOROACETIC ACID		
C3H6O2	PROPIONIC ACID		50
		C6H6 BENZENE	278-279
C6H6	BENZENE		51
C2H3CLO2	CHLOROACETIC ACID		
C2H4O2	ACETIC ACID		52- 53
C2H4O2	ACETIC ACID		
			54-60 60 R
CCL4	TETRACHLOROMETHANE		54-60 60 R
		C6H15N TRIETHYLAMINE	280-281
CHCL3	CHLOROFORM		61- 63
		CH2O2 FORMIC ACID	273-274

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
C2H4O2	ACETIC ACID			
CH2CL2	DICHLOROMETHANE		64- 65	
CH2O2	FORMIC ACID		7- 12	
		C3H6O2	PROPIONIC ACID	275-277
C2HCL3	TRICHLOROETHYLENE		66- 73 73	
C2H3CLO2	CHLOROACETIC ACID		52- 53	
C2H4CL2	1,2-DICHLOROETHANE		74- 76	
C2H5NO	ACETAMIDE		77	
C3H4O2	ACRYLIC ACID		78- 80	
C3H5CL	3-CHLORO-1-PROPENE		81	
C3H6O2	METHYL ACETATE		82- 83	
C3H6O2	PROPIONIC ACID		84- 86	
		C4H8O2	BUTYRIC ACID	282
C3H7CL	1-CHLOROPROPANE		87	
C3H7CL	ISOPROPYL CHLORIDE		88	
C4H5N	METHACRYLONITRILE		89	
C4H6O2	VINYL ACETATE		90- 95	
C4H6O3	ACETIC ANHYDRIDE		96-102	
		C5H8O4	METHYLENE DIACETATE	283-284
		C6H6	BENZENE	285-286
C4H8O2	BUTYRIC ACID		103	
C4H8O2	ETHYL ACETATE		104-108	
		C5H8O2	ETHYL ACRYLATE	287
		C6H14	HEXANE	288
C4H9CL	BUTYL CHLORIDE		109	
C4H9CL	TERT-BUTYL CHLORIDE		110	
C4H9CL	ISOBUTYL CHLORIDE		111	
C4H9NO	N,N-DIMETHYLACETAMIDE		112-116 116	
C5H5N	PYRIDINE		117-118	
C5H8O2	ALLYL ACETATE		119	
C5H8O2	ETHYL ACRYLATE		120	
C5H8O4	METHYLENE DIACETATE		121	
C5H10	2-METHYL-2-BUTENE		122	
C5H10O2	ISOPROPYL ACETATE		123	
C5H10O2	PROPYL ACETATE		124	
C5H12	2-METHYLBUTANE		125	
C6H6	BENZENE		126-145 145	
		C6H12	CYCLOHEXANE	289

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE
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C6H12	CYCLOHEXANE		146
C6H12O2	BUTYL ACETATE		147-151
		C7H14O2 ISOPENTYL ACETATE	290
C6H14	HEXANE		152-153
C6H15N	TRIETHYLAMINE		154-156
C6H18OSi2	HEXAMETHYLDISILOXANE		157-158
C7H8	TOLUENE		159-168 168 R
		C7H16 HEPTANE	291-292
C7H9N	2,6-DIMETHYLPYRIDINE		169
		C10H22 DECANE	293
C7H14O2	ISOPENTYL ACETATE		170-172
C7H16	HEPTANE		173-176
C8H8	STYRENE		177
		C8H10 ETHYLBENZENE	294
C8H10	ETHYLBENZENE		178-179
C8H10	O-XYLENE		180
C8H10	P-XYLENE		181-182
C8H11N	N,N-DIMETHYLANILINE		183
C8H14O2	CYCLOHEXYL ACETATE		184
C8H14O4	2,3-BUTANEDIOL DIACETATE		185-188 188 R
C8H18	OCTANE		189-190
C10H22	DECANE		191
C2H4O2	METHYL FORMATE		
CH4S	METHANETHIOL		309
C3H7NO	N,N-DIMETHYLFORMAMIDE		310-326 326 R
C5H8	ISOPRENE		327
C5H10	2-METHYL-2-BUTENE		328
C6H14	HEXANE		329
C3H4O2	ACRYLIC ACID		
CH2O2	FORMIC ACID		13
C2H2CL2	1,1-DICHLOROETHYLENE		192
C2H4O2	ACETIC ACID		78-80
C4H6O2	VINYL ACETATE		193
C5H10O2	ISOPROPYL ACETATE		194
C8H8	STYRENE		195-201

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
C3H6O2	ETHYL FORMATE			
CHCL3	CHLOROFORM		330-331	
C2H2CL2	CIS-1,2-DICHLOROETHYLENE		332	
C2H2CL2	TRANS-1,2-DICHLOROETHYLENE		333	
C3H6O2	METHYL ACETATE		334	
C6H6	BENZENE		335-336	
C6H12	CYCLOHEXANE		337-338	
C3H6O2	METHYL ACETATE			
CCL4	TETRACHLOROMETHANE		339-340	
CHCL3	CHLOROFORM		341-346 346 R	
		C6H6	BENZENE	660-664
CH2CL2	DICHLOROMETHANE		347	
CH3I	METHYL IODIDE		348	
CS2	CARBON DISULFIDE		349-350	
C2H2CL2	CIS-1,2-DICHLOROETHYLENE		351	
C2H2CL2	TRANS-1,2-DICHLOROETHYLENE		352	
C2H3N	ACETONITRILE		353-354	
C2H4O2	ACETIC ACID		82- P3	
C3H6O2	ETHYL FORMATE		334	
C4H6O2	VINYL ACETATE		355	
C4H6O3	ACETIC ANHYDRIDE		299	
C4H8O2	ETHYL ACETATE		356-370	
C5H10O2	PROPYL ACETATE		371-373	
C6H5CL	CHLOROBENZENE		374	
C6H6	BENZENE		375-390 390 R	
		C6H12	CYCLOHEXANE	665-666
C6H12	CYCLOHEXANE		391-394 394 R	
C6H12	1-HEXENE		395	
C6H12O2	BUTYL ACETATE		396-397	
C7H14O2	PENTYL ACETATE		398-401	
C3H6O2	PROPIONIC ACID			
CCL4	TETRACHLOROMETHANE		202-208	
CH2O2	FORMIC ACID		14- 16	
		C2H4O2	ACETIC ACID	275-277
C2HF3O2	TRIFLUOROACETIC ACID		50	
		C6H6	BENZENE	278-279

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1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
C3H6O2	PROPIONIC ACID			
C2H4O2	ACETIC ACID		84-86	
		C4H8O2	BUTYRIC ACID	282
C6H5Cl	CHLOROBENZENE		209	
C6H6	BENZENE		210-211	
C6H12	CYCLOHEXANE		212	
C6H18OSi2	HEXAMETHYLDISILOXANE		213-214	
C7H16	HEPTANE		215	
C8H10	ETHYLBENZENE		216	
C8H10	M-XYLENE		217	
C8H10	O-XYLENE		218	
C8H10	P-XYLENE		219	
C8H18	OCTANE		220-221	
C9H12	ISOPROPYLBENZENE		222	
C3H6O3	DIMETHYL CARBONATE			
C6H10	1-HEXYNE		402-404	
C7H8	TOLUENE		405	
C7H14	METHYLCYCLOHEXANE		406	
C3H9BO3	METHYL BORATE			
CCL4	TETRACHLOROMETHANE		407	
C6H6	BENZENE		408	
C4H2O3	MALEIC ANHYDRIDE			
C8H10	O-XYLENE		297	
C4H6O2	METHACRYLIC ACID			
C2H2Cl2	1,1-DICHLOROETHYLENE		223	
C4H6O2	VINYL ACETATE		224	
C5H8O2	METHYL METHACRYLATE		225	
C8H14O2	BUTYL METHACRYLATE		226	
C4H6O2	METHYL ACRYLATE			
C4H6O2	VINYL ACETATE		409	
C7H8	TOLUENE		410	
C8H8	STYRENE		411	
C8H10	ETHYLBENZENE		412	
C8H10	M-XYLENE		413	

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
C4H6O2	METHYL ACRYLATE			
C8H1C	O-XYLENE		414	
C8H1C	P-XYLENE		415	
C9H12	ISOPROPYLBENZENE		416	
C9H12	1,3,5-TRIMETHYLBENZENE		417	
C4H6O2	VINYL ACETATE			
C2H2CL2	1,1-DICHLOROETHYLENE		418	
C2H4O2	ACETIC ACID		90-95	
C3H3N	ACRYLONITRILE		419-420	
C3H4O2	ACRYLIC ACID		193	
C3H6O2	METHYL ACETATE		355	
C4H6O2	METHACRYLIC ACID		224	
C4H6O2	METHYL ACRYLATE		409	
C5H8O2	ALLYL ACETATE		421	
C5H8O2	METHYL METHACRYLATE		422	
C6H12	CYCLOHEXANE		423	
C6H12	1-HEXENE		424-426 426 R	
C6H14	HEXANE		427-430 430 R	
C7H16	2,4-DIMETHYLPENTANE		431	
C4H6O3	ACETIC ANHYDRIDE			
CH3I	METHYL IODIDE		298	
C2H4O2	ACETIC ACID		96-102	
		C5H8O4	METHYLENE DIACETATE	283-284
		C6H6	BENZENE	285-286
C3H6O2	METHYL ACETATE		299	
C5H5N	PYRIDINE		300	
C5H8O2	ISOPROPENYL ACETATE		301	
C5H8O4	METHYLENE DIACETATE		302-304	
C6H6	BENZENE		305	
C6H12	CYCLOHEXANE		306	
C4H6O3	PROPYLENE CARBONATE			
C2H6S	ETHANETHIOL		432-435	
C4H8O2	BUTYRIC ACID			
CH2CL2	DICHLOROMETHANE		227	
CH2O2	FORMIC ACID		28	

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C4H8O2	BUTYRIC ACID			
C2H4O2	ACETIC ACID		103	
		C3H6O2	PROPIONIC ACID	282
C5H10O2	VALERIC ACID		228	
C6H18OSi2	HEXAMETHYLDISILOXANE		229-230	
C8H10	P-XYLENE		231	
C8H10	O-XYLENE		232	
C8H10	F-XYLENE		233	
C8H11N	N,N-DIMETHYLANILINE		234	
C8H18	OCTANE		235	
C9H12	ISOPROPYLBENZENE		236	
C10H15N	N,N-DIETHYLANILINE		237	
C4H8O2	ETHYL ACETATE			
CCL4	TETRACHLOROMETHANE		436-442 442 R	
CHCL3	CHLOROFORM		443-448 448 R	
CH2CL2	DICHLOROMETHANE		449	
C2HCL3	TRICHLOROETHYLENE		450-454	
C2H3N	ACETONITRILE		455-458	
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		C5H8O2	ETHYL ACRYLATE	287
		C6H14	HEXANE	288
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C2H6OS	DIMETHYL SULFOXIDE		460-461	
C3H6O2	METHYL ACETATE		356-370	
C4H9NO	METHYL ETHYL KETOXIM		462	
C4H11N	DIETHYLAMINE		463-486 486 R	
C5H10O2	ISOPROPYL ACETATE		487	
C6H5Cl	CHLOROBENZENE		488-492	
C6H6	BENZENE		493-504 504 R	
		C6H12	CYCLOHEXANE	667-668
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C6H12	CYCLOHEXANE		506-509 509 R	
C6H12	1-HEXENE		510-513 513 R	
C6H14	HEXANE		514-515	
C7H8	TOLUENE		516-530	

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1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	PAGE	
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	C7H14O2	PENTYL ACETATE	531-537	
	C8H10	ETHYLBENZENE	536-540	
	C8H10	P-XYLENE	541	
	C8H16	1-OCTENE	542	
C4H8O2	ISOBUTYRIC ACID			
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	BUTYL FORMATE	C5H10O2	565
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