J. Gmehling
U. Onken
W. Arlt

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

Aqueous-Organic Systems (Supplement 1)

Chemistry Data Series

Vol. I, Part 1a

Published by DECHEMA
Deutsche Gesellschaft für Chemisches Apparatewesen,
Chemische Technik und Biotechnologie e.V.

Executive Editor: Gerhard Kreysa

Vapor-Liquid Equilibrium Data Collection

1a

Aqueous-Organic Systems (Supplement 1)

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, W. Arlt

Universität Oldenburg
Universität Dortmund
Technische Universität Berlin

Die Deutsche Bibliothek – CIP-Einheitsaufnahme

Chemistry data series / publ. by DECHEMA, Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik und Biotechnologie e.V. Executive ed.: Gerhard Kreysa. – Frankfurt am Main: DECHEMA

Teilw. hrsg. von DECHEMA, Deutsche Gesellschaft für Chemisches Apparatewesen. – Teilw. hrsg. von Dieter Behrens und Reiner Eckermann. – Teilw. hrsg. von Reiner Eckermann und Gerhard Kreysa.

Vol. I Vapor liquid equilibrium data collection
Pt. 1a. Aqueous organic systems. – (Suppl. 1). Tables and diagrams of data for binary and multicomponent mixtures up to moderate pressures; constants of correlation equations for computer use. – 2. ed. with minor changes and corr. – 1998

Vapor liquid equilibrium data collection / publ. by DECHEMA, Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik und Biotechnologie e.V. – Frankfurt am Main: DECHEMA
(Chemistry data series; Vol. I)
Teilw. hrsg. von DECHEMA, Deutsche Gesellschaft für Chemisches Apparatewesen.

Pt. 1a. Aqueous organic systems. – (Suppl. 1). 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; W. Arlt. – 2. ed. with minor changes and corr. – 1998

ISBN 3-926959-90-8

This volume of the Chemistry Data Series was printed using acid-free paper.

Printed by Brönners Druckerei Breidenstein GmbH, Frankfurt am Main, Germany

1a

Aqueous-Organic Systems (Supplement 1)

Systems with:

Deuterium oxide
Water

AUTHORS' PREFACE

With this part 1a we present the first supplement of our Vapor-Liquid Equilibrium Data Collection; supplements to part 2 are in preparation. These supplements will contain mainly data published after completion of the respective volume. Besides, older data from sources not accessible to us before will be included at this occasion. Likewise the supplements will additionally contain so-called incomplete x-y data at constant temperature without experimental data for the pressure. Finally, coming to the so-called recommended values for the constants of Wilson, NRTL, and UNIQUAC equations (see Guide to Tables, p. XXVI), it should be remembered, that these are given from part 3/4 onwards. In the supplements 1 and 2 we therefore have included recommended values for systems of parts 1, 2a and 2b. In some cases, especially for systems with large mixing enthalpies, fitting could be improved by using a linear relationship with temperature for the parameters; otherwise, recommended parameters are given as independent on temperature.

Again we should like to thank all colleagues who have supplied us with experimental VLE data from their laboratories by sending us reprints, especially to Dr. L. S. Kudrjawzewa (Estonian Academy of Science, Tallinn) and to Prof. Dr. H.-J. Bittrich (T.H. Leuna-Merseburg)

On this occasion we should like to recall that our data collection is the result of the diligent and devoted work of many people at the University of Dortmund. The following persons have contributed to this volume: Mrs. U. Arlt, Mrs. A. Brunk, Dipl.-Ing. P. Grenzheuser, Dipl.-Ing. B. Kolbe, Mrs. L. Kunzner, cand.-chem. J. Menke, Dr. G. Nocon, Mrs. G. Obermann, and Dipl.-Chem. U. Weidlich from our team, and Mr. T. Blaszyk from the computer center.

Dortmund, October 1981

Ulfert Onken Jürgen Gmehling Wolfgang Arlt

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. 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 1981

Dieter Behrens
Reiner Eckermann

CONTENTS
Vol. I, Part 1a

R = RECOMMENDED VALUES

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT		PAGE
D2O	DEUTERIUM OXIDE			
	C3H6O2 DIOXOLANE			1
	C4H8O TETRAHYDROFURAN			2- 4 4 R
H2O	WATER			
	CHCL3 CHLOROFORM	C2H6O	ETHANOL	469
	CHN HYDROGEN CYANIDE			5- 6
	CH2CL2 DICHLOROMETHANE	CH4O	METHANOL	470
		C2H4O2	ACETIC ACID	471
		C4H8O	2-BUTANONE	472
	CH2O FORMALDEHYDE			7- 33
		CH4O	METHANOL	473-480
	CH2O2 FORMIC ACID			34- 41
		C2H4O2	ACETIC ACID	481-490
		C3H8O C4H8O2	2-PROPANOL ISOPROPYL FORMATE	680
		C6H12O2	ISOPENTYL FORMATE	491
	CH3NO2 NITROMETHANE			42- 45
		C3H8O	2-PROPANOL	492
		C6H14O	1-HEXANOL	493
	CH4O METHANOL			46- 63 62- 63 R
		C2H6O	ETHANOL	494-495
		C3H6O	ACETONE	496-500
		C3H6O2	METHYL ACETATE	501
		C3H6O2 C4H6O2	METHYL ACETATE VINYL ACETATE	681-682
		C3H8O	1-PROPANOL	502-503
		C3H8O	2-PROPANOL	504-506
		C4H6O2	METHYL ACRYLATE	507-508
		C4H10O	1-BUTANOL	509
		C4H10O	TERT-BUTANOL	510
		C5H4O2	FURFURAL	511-513
		C5H8O2	METHYL METHACRYLATE	514
		C5H12O	1-PENTANOL	515
		C6H12O2	BUTYL ACETATE	516
		C7H6O2	BENZOIC ACID	517
	C2H2CL4 1,1,2,2-TETRACHLOROETHANE			64

Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT		PAGE
H2O	WATER			
	C4H8O	TETRAHYDROFURAN		282-286 286 R
		C6H14	HEXANE	647
	C4H8O2	BUTYRIC ACID		287
		C5H10O	3-PENTANONE	648
	C4H8O2	1,4-DIOXANE		288-303 303 R
	C4H8O2	ETHYL ACETATE		304-306 306 R
		C6H6 C6H12O2	BENZENE BUTYL ACETATE	685-686
		C6H12O2	BUTYL ACETATE	649
	C4H8O2	ISOBUTYRIC ACID	C4H10O 2-BUTANOL	650
	C4H8O2S	SULFOLANE		307-316
	C4H9NO	N,N-DIMETHYLACETAMIDE		317-325
	C4H9NO	MORPHOLINE		326-327
	C4H10O	1-BUTANOL		328-336 336 R
		C4H10O	2-METHYL-1-PROPANOL	651-653
		C5H12O	TERT-PENTANOL	654-655
		C6H12O2	BUTYL ACETATE	656
		C6H12O2 C7H14O2	BUTYL ACETATE ISOPENTYL ACETATE	687-688
		C7H8	TOLUENE	657
		C7H14O2	ISOPENTYL ACETATE	658
		C8H18O	DIBUTYL ETHER	659
	C4H10O	2-BUTANOL		337-339
		C4H10O	TERT-BUTANOL	660
		C8H16	2,4,4-TRIMETHYL-1-PENTENE	661
	C4H10O	TERT-BUTANOL		340-343
		C8H16	2,4,4-TRIMETHYL-1-PENTENE	662
	C4H10O	DIETHYL ETHER		344
	C4H10O	2-METHYL-1-PROPANOL		345
		C7H8	TOLUENE	663-664
	C4H10O2	1,4-BUTANEDIOL		346-347
	C4H10O2	2,3-BUTANEDIOL		348-351 351 R
	C4H10O3	DIETHYLENE GLYCOL		352-353
	C4H11N	BUTYLAMINE		354-355 355 R
	C5H4O2	FURFURAL		356-361

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT		PAGE
H2O	WATER			
	C5H5N PYRIDINE			362-374 374 R
	C5H8 ISOPRENE	C5H10	2-METHYL-2-BUTENE	665
	C5H8O METHYL CYCLOPROPYL KETONE			375
	C5H9NO N-METHYLPYRROLIDONE			376-380 380 R
	C5H10O 2-METHYL-3-BUTEN-2-OL			381
	C5H12O 3-METHYLBUTANOL			382
	C5H12O 1-PENTANOL			383
	C5H12O TERT-PENTANOL			384
	C5H13N DIMETHYLISOPROPYLAMINE			385-388
	C5H13N ETHYLISOPROPYLAMINE			389-392
	C5H13N METHYLDIETHYLAMINE			393 R
	C6H6 BENZENE	C6H12O2	BUTYL ACETATE	666
		C8H8	STYRENE	667
		C8H10	ETHYLBENZENE	668
	C6H6O PHENOL			394-399 399 R
		C6H10O	CYCLOHEXANONE	669-670
		C6H10O	MESITYLOXIDE	671-672
		C6H12O2	BUTYL ACETATE	673
		C6H15N	TRIETHYLAMINE	674-675
		C7H16	HEPTANE	676
	C6H7N ANILINE			400-401
	C6H7N 2-METHYLPYRIDINE			402-404
	C6H7N 3-METHYLPYRIDINE			405-406 406 R
	C6H7N 4-METHYLPYRIDINE			407-408
	C6H8N2 PHENYLHYDRAZINE			409
	C6H10O CYCLOHEXANONE			410
	C6H10O MESITYLOXIDE			411
	C6H10O METHYLDIHYDROPYRAN			412
	C6H12O CYCLOHEXANOL			413-416
	C6H12O2 BUTYL ACETATE			417-418 418 R
		C7H14O2	ISOPENTYL ACETATE	677
	C6H12O2 DIACETONE ALCOHOL			419 R
	C6H12O2 PROPYL PROPIONATE			420

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT		PAGE
H2O	WATER			
C6H14O	DIISOPROPYL ETHER			421
C6H14O	1-HEXANOL			422-426
C6H14O	2-HEXANOL			427
C6H14O2	2-BUTOXYETHANOL			428-433 433 R
C6H15N	ETHYLBUTYLAMINE			434-436
C6H15N	N-ETHYL-SEC-BUTYLAMINE			437-442
C6H15N	TRIETHYLAMINE			443-445
C7H6O2	BENZOIC ACID			446
		C12H10	BIPHENYL	678
C7H8O	BENZYL ALCOHOL			447-450
C7H8O	2-METHYLPHENOL			451
C7H8O	3-METHYLPHENOL			452
C7H8O	4-METHYLPHENOL			453
C7H8O2	GUIACOL			454
C7H9N	2,4-DIMETHYLPYRIDINE			455
C7H9N	2,6-DIMETHYLPYRIDINE			456-458
C7H14O2	ISOPENTYL ACETATE			459
C8H8	STYRENE	C8H10	ETHYLBENZENE	679
C8H8O	ACETOPHENONE			460
C8H11N	2-METHYL-5-ETHYLPYRIDINE			461
C9H7N	QUINOLINE			462-464
C9H12	ISOPROPYLBENZENE			465
C10H14N2	NICOTINE			466-468

1ST COMPONENT	2ND COMPONENT		3RD COMPONENT 4TH COMPONENT		PAGE
WATER		H2O			
	ACRYLONITRILE	C3H3N			180-183
			ACETONE	C3H6O	583-585
			ACROLEIN	C3H4O	579-581
			PROPIONITRILE	C3H5N	582
	ALLYL ALCOHOL	C3H6O			203-208
			2-PROPANOL	C3H8O	600-601
	ANILINE	C6H7N			400-401
	BENZENE	C6H6	BUTYL ACETATE	C6H12O2	666
			ETHYLBENZENE	C8H10	668
			STYRENE	C8H8	667
	BENZOIC ACID	C7H6O2			446
			BIPHENYL	C12H10	678
	BENZYL ALCOHOL	C7H8O			447-450
	1,4-BUTANEDIOL	C4H10O2			346-347
	2,3-BUTANEDIOL	C4H10O2			348-351 351 R
	1-BUTANOL	C4H10O			328-336 336 R
			BUTYL ACETATE	C6H12O2	656
			BUTYL ACETATE ISOPENTYL ACETATE	C6H12O2 C7H14O2	687-688
			DIBUTYL ETHER	C8H18O	659
			ISOPENTYL ACETATE	C7H14O2	658
			2-METHYL-1-PROPANOL	C4H10O	651-653
			TERT-PENTANOL	C5H12O	654-655
			TOLUENE	C7H8	657
	2-BUTANOL	C4H10O			337-339
			TERT-BUTANOL	C4H10O	660
			2,4,4-TRIMETHYL-1-PENTENE	C8H16	661
	TERT-BUTANOL	C4H10O			340-343
			2,4,4-TRIMETHYL-1-PENTENE	C8H16	662
	2-BUTANONE	C4H8O			271-279 279 R
			BENZENE	C6H6	641-642
			1-BUTANOL	C4H10O	632
			2-BUTANOL	C4H10O	633-640
			2-BUTOXYETHANOL	C6H14O2	644
			DIISOPROPYL ETHER	C6H14O	643
			TETRAHYDROFURAN	C4H8O	630-631

1ST COMPONENT	2ND COMPONENT		3RD COMPONENT 4TH COMPONENT		PAGE
WATER		H2O			
	2-BUTOXYETHANOL	C6H14O2			428-433 433 R
	BUTYL ACETATE	C6H12O2			417-418 418 R
			ISOPENTYL ACETATE	C7H14O2	677
	BUTYLAMINE	C4H11N			354-355 355 R
	BUTYRALDEHYDE	C4H8O	ISOBUTYRALDEHYDE	C4H8O	645-646
	BUTYRIC ACID	C4H8O2			287
			3-PENTANONE	C5H10O	648
	2-CHLOROETHANOL	C2H5CLO			110-113
	CHLOROFORM	CHCL3	ETHANOL	C2H6O	469
	3-CHLORO-1-PROPENE	C3H5CL			188
	CYCLOHEXANOL	C6H12O			413-416
	CYCLOHEXANONE	C6H10O			410
	DIACETONE ALCOHOL	C6H12O2			419 R
	1,2-DICHLOROETHANE	C2H4CL2	ACETIC ACID	C2H4O2	522
	DICHLOROMETHANE	CH2CL2	ACETIC ACID	C2H4O2	471
			2-BUTANONE	C4H8O	472
			METHANOL	CH4O	470
	DIETHYLENE GLYCOL	C4H10O3			352-353
	DIETHYL ETHER	C4H10O			344
	DIISOPROPYL ETHER	C6H14O			421
	DIMETHOXYMETHANE	C3H8O2			252
	N,N-DIMETHYLACETAMIDE	C4H9NO			317-325
	DIMETHYLAMINE	C2H7N			174-176
	N,N-DIMETHYLFORMAMIDE	C3H7NO			227-234 234 R
			TETRAHYDROFURAN	C4H8O	603
	DIMETHYLISOPROPYL- AMINE	C5H13N			385-388
	2,4-DIMETHYLPYRIDINE	C7H9N			455
	2,6-DIMETHYLPYRIDINE	C7H9N			456-458
	DIMETHYL SULFOXIDE	C2H6OS			158-165 165 R
	1,4-DIOXANE	C4H8O2			288-303 303 R
	DIOXOLANE	C3H6O2			210-213 213 R
	1,2-ETHANEDIOL	C2H6O2			166-173

1ST COMPONENT	2ND COMPONENT		3RD COMPONENT 4TH COMPONENT		PAGE
WATER		H2O			
	ETHANOL	C2H6O			116-157 156-157 R
			ACETONE	C3H6O	546-547
			ALLYL ALCOHOL	C3H6O	548
			BENZENE	C6H6	572-577
			BENZENE HEPTANE	C6H6 C7H16	684
			1-BUTANOL	C4H10O	563-565
			TERT-BUTANOL	C4H10O	566
			BUTYL ACETATE	C6H12O2	578
			BUTYRALDEHYDE	C4H8O	554-555
			1,4-DIOXANE	C4H8O2	556-559
			ETHYL ACETATE	C4H8O2	560-562
			FURFURAL	C5H4O2	568
			METHYL ACETATE	C3H6O2	549
			3-METHYLBUTANOL	C5H12O	569-571
			2-METHYL-1-PROPANOL	C4H10O	567
			1-PROPANOL	C3H8O	550-551
			2-PROPANOL	C3H8O	552-553
	ETHYL ACETATE	C4H8O2			304-306 306 R
			BENZENE BUTYL ACETATE	C6H6 C6H12O2	685-686
			BUTYL ACETATE	C6H12O2	649
	ETHYLAMINE	C2H7N			177
	ETHYLBUTYLAMINE	C6H15N			434-436
	N-ETHYL-SEC-BUTYLAMINE	C6H15N			437-442
	ETHYLENEDIAMINE	C2H8N2			178-179 179 R
	ETHYLENE OXIDE	C2H4O			87- 88
	ETHYLISOPROPYLAMINE	C5H13N			389-392
	FORMALDEHYDE	CH2O			7- 33
			METHANOL	CH4O	473-480
	FORMIC ACID	CH2O2			34- 41
			ACETIC ACID	C2H4O2	481-490
			ISOPENTYL FORMATE	C6H12O2	491
			ISOPROPYL FORMATE 2-PROPANOL	C4H8O2 C3H8O	680
	FURFURAL	C5H4O2			356-361
	GLYCEROL	C3H8O3			265
	GUIACOL	C7H8O2			454

1ST COMPONENT	2ND COMPONENT		3RD COMPONENT 4TH COMPONENT		PAGE
WATER	H2O				
	1-HEXANOL	C6H14O			422-426
	2-HEXANOL	C6H14O			427
	HYDROGEN CYANIDE	CHN			5- 6
	ISOBUTYRALDEHYDE	C4H8O			280-281
	ISOBUTYRIC ACID	C4H8O2	2-BUTANOL	C4H10O	650
	ISOPENTYL ACETATE	C7H14O2			459
	ISOPRENE	C5H8	2-METHYL-2-BUTENE	C5H10	665
	ISOPROPYLAMINE	C3H9N			266
			DIISOPROPYLAMINE	C6H15N	629
	ISOPROPYLBENZENE	C9H12			465
	MESITYLOXIDE	C6H10O			411
	METHANOL	CH4O			46- 63 62- 63 R
			ACETONE	C3H6O	496-500
			BENZOIC ACID	C7H6O2	517
			1-BUTANOL	C4H10O	509
			TERT-BUTANOL	C4H10O	510
			BUTYL ACETATE	C6H12O2	516
			ETHANOL	C2H6O	494-495
			FURFURAL	C5H4O2	511-513
			METHYL ACETATE	C3H6O2	501
			METHYL ACETATE VINYL ACETATE	C3H6O2 C4H6O2	681-682
			METHYL ACRYLATE	C4H6O2	507-508
			METHYL METHACRYLATE	C5H8O2	514
			1-PENTANOL	C5H12O	515
			1-PROPANOL	C3H8O	502-503
			2-PROPANOL	C3H8O	504-506
	2-METHOXYPROPIONITRILE	C4H7NO			268-270
	N-METHYLACETAMIDE	C3H7NO			235
	METHYL ACETATE	C3H6O2			214 R
	3-METHYLBUTANOL	C5H12O			382
	2-METHYL-3-BUTEN-2-OL	C5H10O			381
	METHYL CYCLOPROPYL-KETONE	C5H8O			375
	METHYLDIETHYLAMINE	C5H13N			393 R
	METHYLDIHYDROPYRAN	C6H10O			412
	2-METHYL-5-ETHYL-PYRIDINE	C8H11N			461

1ST COMPONENT	2ND COMPONENT		3RD COMPONENT 4TH COMPONENT		PAGE
WATER		H2O			
	N-METHYLFORMAMIDE	C2H5NO			114-115 115 R
	2-METHYLPHENOL	C7H8O			451
	3-METHYLPHENOL	C7H8O			452
	4-METHYLPHENOL	C7H8O			453
	2-METHYL-1-PROPANOL	C4H10O			345
			TOLUENE	C7H8	663-664
	2-METHYLPYRIDINE	C6H7N			402-404
	3-METHYLPYRIDINE	C6H7N			405-406 406 R
	4-METHYLPYRIDINE	C6H7N			407-408
	N-METHYLPYRROLIDONE	C5H9NO			376-380 380 R
	MORPHOLINE	C4H9NO			326-327
	NICOTINE	C10H14N2			466-468
	NITROMETHANE	CH3NO2			42- 45
			1-HEXANOL	C6H14O	493
			2-PROPANOL	C3H8O	492
	1-PENTANOL	C5H12O			383
	TERT-PENTANOL	C5H12O			384
	PHENOL	C6H6O			394-399 399 R
			BUTYL ACETATE	C6H12O2	673
			CYCLOHEXANONE	C6H10O	669-670
			HEPTANE	C7H16	676
			MESITYLOXIDE	C6H10O	671-672
			TRIETHYLAMINE	C6H15N	674-675
	PHENYLHYDRAZINE	C6H8N2			409
	1,2-PROPANEDIOL	C3H8O2			253-264
	1-PROPANOL	C3H8O			236-240 240 R
			BENZENE	C6H6	606-608
			1-BUTANOL	C4H10O	604-605
			BUTYL ACETATE	C6H12O2	609
			PROPYL PROPIONATE	C6H12O2	610
	2-PROPANOL	C3H8O			241-251 251 R
			BENZENE	C6H6	612-625
			2-BUTANONE	C4H8O	611
			CYCLOHEXANE	C6H12	626
			TOLUENE	C7H8	627-628

1ST COMPONENT	2ND COMPONENT		3RD COMPONENT 4TH COMPONENT		PAGE
WATER		H2O			
	PROPIONALDEHYDE	C3H6O			209
	PROPIONIC ACID	C3H6O2			215-224
			3-PENTANONE	C5H10O	602
	PROPIONITRILE	C3H5N			189
	PROPYLAMINE	C3H9N			267
	PROPYL PROPIONATE	C6H12O2			420
	PYRIDINE	C5H5N			362-374 374 R
	QUINOLINE	C9H7N			462-464
	STYRENE	C8H8	ETHYLBENZENE	C8H10	679
	SULFOLANE	C4H8O2S			307-316
1,1,2,2-TETRACHLOROETHANE		C2H2CL4			64
	TETRAHYDROFURAN	C4H8O			282-286 286 R
			HEXANE	C6H14	647
	THIAZOLE	C3H3NS			184
	TRIETHYLAMINE	C6H15N			443-445
1,3,5-TRIOXANE		C3H6O3			225-226