

**J. Gmehling  
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W. Arlt**

# **VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION**

**Aqueous-Organic Systems  
(Supplement 1)**



## **Chemistry Data Series**

**Vol. I, Part 1a**

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**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**

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– Teilw. hrsg. von Dieter Behrens und Reiner Eckermann. – Teilw. hrsg. von Reiner Eckermann und Gerhard Kreysa.

Vol. I Vapor liquid equilibrium data collection

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**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. Grenzeuser, 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

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## Formula Index of Systems

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
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		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 2-PROPANOL	
-----			
		C4H8O2 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 METHYL ACETATE	
-----			
		C4H6O2 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			
C2H3N	ACETONITRILE		65-76 76 R	
		C2H6O	ETHANOL	518-519
		C3H3N	ACRYLONITRILE	520-521
C2H4CL2	1,2-DICHLOROETHANE	C2H4O2	ACETIC ACID	522
C2H4O	ACETALDEHYDE		77-86 86 R	
		C2H4O2	ACETIC ACID	523-526
		C2H6O	ETHANOL	527
		C4H10O	DIETHYL ETHER	528
C2H4O	ETHYLENE OXIDE		87-88	
C2H4O2	ACETIC ACID		89-109	
		C3H6O	ACETONE	529
		C3H6O2	METHYL ACETATE	530
		C3H6O2	PROPIONIC ACID	531
		C4H6O2	VINYL ACETATE	532-534
		C4H6O3	ACETIC ANHYDRIDE	535
		C4H8O	2-BUTANONE	536-538
		C4H8O	2-BUTANONE	
		C6H14O	DIISOPROPYL ETHER	683
		C5H10O2	ISOPROPYL ACETATE	539
		C6H12O2	BUTYL ACETATE	540-542
		C7H8	TOLUENE	543
		C8H10	P-XYLENE	544
		C8H18O	2-ETHYL-1-HEXANOL	545
C2H5ClO	2-CHLOROETHANOL		110-113	
C2H5NO	N-METHYLFORMAMIDE		114-115 115 R	
C2H6O	ETHANOL		116-157 156-157 R	
		C3H6O	ACETONE	546-547
		C3H6O	ALLYL ALCOHOL	548
		C3H6O2	METHYL ACETATE	549
		C3H8O	1-PROPANOL	550-551
		C3H8O	2-PROPANOL	552-553
		C4H8O	BUTYRALDEHYDE	554-555
		C4H8O2	1,4-DIOXANE	556-559
		C4H8O2	ETHYL ACETATE	560-562
		C4H10O	1-BUTANOL	563-565

## Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE
H2O	WATER		
C2H6O	ETHANOL	C4H100 TERT-BUTANOL	566
		C4H100 2-METHYL-1-PROPANOL	567
		C5H4O2 FURFURAL	568
		C5H120 3-METHYLBUTANOL	569-571
		C6H6 BENZENE	572-577
		C6H6 BENZENE	
		C7H16 HEPTANE	684
		C6H12O2 BUTYL ACETATE	578
C2H6OS	DIMETHYL SULFOXIDE		158-165 165 R
C2H6O2	1,2-ETHANEDIOL		166-173
C2H7N	DIMETHYLAMINE		174-176
C2H7N	ETHYLAMINE		177
C2H8N2	ETHYLENEDIAMINE		178-179 179 R
C3H3N	ACRYLONITRILE		180-183
		C3H4O ACROLEIN	579-581
		C3H5N PROPIONITRILE	582
		C3H6O ACETONE	583-585
C3H3NS	THIAZOLE		184
C3H4O2	ACRYLIC ACID		185-187
		C4H6O2 METHYL ACRYLATE	586
		C5H10O2 ISOPROPYL ACETATE	587
		C8H18O 2-ETHYL-1-HEXANOL	588
C3H5CL	3-CHLORO-1-PROPENE		188
C3H5N	PROPIONITRILE		189
C3H6O	ACETONE		190-202 202 R
		C3H8O 2-PROPANOL	589-591
		C4H10O 1-BUTANOL	592-593
		C5H4O2 FURFURAL	594-596
		C5H8O2 METHYL METHACRYLATE	597
		C5H12 PENTANE	598
		C6H14 HEXANE	599
C3H6O	ALLYL ALCOHOL		203-208
		C3H8O 2-PROPANOL	600-601
C3H6O	PROPIONALDEHYDE		209

## Formula Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT	4TH COMPONENT	PAGE
H2O	WATER			
C3H6O2	DIOXOLANE			210-213 213 R
C3H6O2	METHYL ACETATE			214 R
C3H6O2	PROPIONIC ACID			215-224
		C5H10O	3-PENTANONE	602
C3H6O3	1,3,5-TRIOXANE			225-226
C3H7NO	N,N-DIMETHYLFORMAMIDE			227-234 234 R
		C4H8O	TETRAHYDROFURAN	603
C3H7NO	N-METHYLACETAMIDE			235
C3H8O	1-PROPANOL			236-240 240 R
		C4H10O	1-BUTANOL	604-605
		C6H6	BENZENE	606-608
		C6H12O2	BUTYL ACETATE	609
		C6H12O2	PROPYL PROPIONATE	610
C3H8O	2-PROPANOL			241-251 251 R
		C4H8O	2-BUTANONE	611
		C6H6	BENZENE	612-625
		C6H12	CYCLOHEXANE	626
		C7H8	TOLUENE	627-628
C3H8O2	DIMETHOXYMETHANE			252
C3H8O2	1,2-PROPANEDIOL			253-264
C3H8O3	GLYCEROL			265
C3H9N	ISOPROPYLAMINE			266
		C6H15N	DIISOPROPYLAMINE	629
C3H9N	PROPYLAMINE			267
C4H7NO	2-METHOXYPROPIONITRILE			268-270
C4H8O	2-BUTANONE			271-279 279 R
		C4H8O	TETRAHYDROFURAN	630-631
		C4H10O	1-BUTANOL	632
		C4H10O	2-BUTANOL	633-640
		C6H6	BENZENE	641-642
		C6H14O	DIISOPROPYL ETHER	643
		C6H14O2	2-BUTOXYETHANOL	644
C4H8O	BUTYRALDEHYDE	C4H8O	ISOBUTYRALDEHYDE	645-646
C4H8O	ISOBUTYRALDEHYDE			280-281

## 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	BENZENE	
		C6H12O2	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	BUTYL ACETATE	
		C7H14O2	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	

## Formula Index of Systems

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	DIMETHYL ISOPROPYLAMINE		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

## Formula Index of Systems

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	GUAIACOL		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



## Alphabetical Index of Systems

1ST COMPONENT	2ND COMPONENT	3RD COMPONENT 4TH COMPONENT	PAGE	
DEUTERIUM OXIDE		D2O		
	DIOXOLANE	C3H6O2	1	
	TETRAHYDROFURAN	C4H8O	2- 4 4 R	
WATER		H2O		
	ACETALDEHYDE	C2H4O	77- 86 86 R	
		ACETIC ACID	C2H4O2	523-526
		DIETHYL ETHER	C4H10O	528
		ETHANOL	C2H6O	527
	ACETIC ACID	C2H4O2	89-109	
		ACETIC ANHYDRIDE	C4H6O3	535
		ACETONE	C3H6O	529
		2-BUTANONE	C4H8O	536-538
		2-BUTANONE DIISOPROPYL ETHER	C4H8O C6H14O	683
		BUTYL ACETATE	C6H12O2	540-542
		2-ETHYL-1-HEXANOL	C8H18O	545
		ISOPROPYL ACETATE	C5H10O2	539
		METHYL ACETATE	C3H6O2	530
		PROPIONIC ACID	C3H6O2	531
		TOLUENE	C7H8	543
		VINYL ACETATE	C4H6O2	532-534
		P-XYLENE	C8H10	544
	ACETONE	C3H6O	190-202 202 R	
		1-BUTANOL	C4H10O	592-593
		FURFURAL	C5H4O2	594-596
		HEXANE	C6H14	599
		METHYL METHACRYLATE	C5H8O2	597
		PENTANE	C5H12	598
		2-PROPANOL	C3H8O	589-591
	ACETONITRILE	C2H3N	65- 76 76 R	
		ACRYLONITRILE	C3H3N	520-521
		ETHANOL	C2H6O	518-519
	ACETOPHENONE	C8H8O	460	
	ACRYLIC ACID	C3H4O2	185-187	
		2-ETHYL-1-HEXANOL	C8H18O	588
		ISOPROPYL ACETATE	C5H10O2	587
		METHYL ACRYLATE	C4H6O2	586



## Alphabetical Index of Systems

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
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	2,3-BUTANEDIOL	C4H10O2	348-351 351 R
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