

**J. Gmehling
U. Onken**

VAPOR-LIQUID EQUILIBRIUM DATA COLLECTION

**Ethers
Supplement 3**

Chemistry Data Series

Vol I, Part 4c

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Vapor-Liquid Equilibrium Data Collection

4c

Ethers

Supplement 3

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

Technische Chemie
Universität Oldenburg

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4c

Ethers (Supplement 3)

bis(2-Chloroethyl) ether
bis(2,2,2-Trifluoroethyl) ether [HFE356MF-F]
Dibutyl ether
Diethylene glycol
Diethylene glycol dimethyl ether
Diethyl ether
2,3-Dihydrofuran
Diisopropyl ether
1,2-Dimethoxyethane
Dimethoxymethane
2,2-Dimethoxypropane
Dimethyl ether
2,2-Dimethyloxirane
1,4-Dioxane
1,3-Dioxolane
Epichlorohydrin
1,2-Epoxybutane
2,3-Epoxy-1-propanol
2-Ethoxyethanol
Ethyl butyl ether
Ethyl tert-butyl ether (ETBE)
Ethylene oxide
Furan
Furfuryl alcohol
2-Methoxyethanol
1-Methoxy-2-propanol
Methyl butyl ether
2-Methylfuran
Methyl tert-amyl ether (TAME)
Methyl tert-butyl ether (MTBE)
2-Methyltetrahydrofuran
Propylene glycol monomethyl ether
1,2-Propylene oxide
Tetrahydrofuran
Tetrahydropyran
Tetrahydropyran-2-one
1,3,5-Trioxane

SUBJECTS OF VOLUME I

The subjects of Volume I in the Chemistry Data Series (CDS) are:

Subtitle	Vol. I, Part
Aqueous Systems	1
	1 a
	1 b
	1 c/d
Organic Hydroxy Compounds	
Alcohols	2 a
Alcohols and Phenols	2 b
	2 c
	2 d
	2 e
	2 f
	2 l/2 m
Alcohols	2 g
	2 h
	2 i
	2 j
	2 k
Aldehydes, Ketones, Ethers	3 + 4
Aldehydes	3 a
	3 c
Ketones	3 b
	3 c
Ethers	4 a
	4 b
	4 c
Carboxylic Acids, Anhydrides, Esters	5
Carboxylic Acids, Anhydrides	5 a
Esters	5 b
Aliphatic Hydrocarbons C ₄ -C ₆	6 a
Aliphatic Hydrocarbons C ₇ -C ₁₈	6 b
	6 c
Aliphatic Hydrocarbons C ₄ -C ₃₀	6 d/e
Aromatic Hydrocarbons	7
	7 a/b
Halogen, Nitrogen, Sulfur and other compounds	8
	8 a

AUTHOR'S PREFACE

This volume is another supplement of our Vapor-Liquid Equilibrium Data Collection. It contains VLE data of systems with ethers from dimethyl ether up to MTBE stored in the Dortmund Data Bank (DDB).

Continuous updating of the Dortmund Data Bank (DDB) is one of main activities of DDBST GmbH (www.ddbst.com). Other activities of this company are the development of software for the synthesis and design of industrial processes and the improvement and expansion of predictive methods, such as UNIFAC, modified UNIFAC and PSRK (www.unifac.org).

Today the Dortmund Data Bank (DDB) is the largest factual data bank for thermophysical properties. It contains all types of pure component properties and mixture data, such as phase equilibria, excess and transport properties for non-electrolyte, electrolyte and polymer systems. The Dortmund Data Bank (DDB) and the software packages for process development are used in-house by a large number of companies. A great part of the stored data is also available online via the online service provided by DECHEMA (<http://dechema.de/en/determ.html>).

The edition of this volume would not have been possible without the valuable efforts of the DDBST team. In particular we thank Jochen Menke for his help during the preparation of this volume. With gratitude we also would like to mention Dr. Richard Sass from DECHEMA for his reliable cooperation in editing this volume.

Oldenburg and Dortmund, November 2012

J. Gmehling U. Onken

EXECUTIVE EDITOR'S PREFACE

DECHEMA e.V. Society for Chemical Engineering and Biotechnology was founded in 1926 with the aim of improving cooperation between chemists and engineers. One concrete implementation of this aim was the publication in the mid-1970s of collections of basic thermophysical data in electronic and book form in response to the increasing importance of mathematical modelling, computer simulation and optimization. On account of its sheer volume and limited circle of interest, this was not the sort of material that publishers rush to publish. DECHEMA leapt into the breach and has since sponsored and published the DECHEMA Chemistry Data Series for well over a quarter of a century. For Volume I, the research work of Prof. Gmehling, Prof. Onken and their co-workers on phase equilibria has been very fruitful. It led to an extension of the UNIFAC methods and has led to the publication of the largest collection of vapor-liquid equilibrium data available at present.

We hope that the publication of this collection of data in the DECHEMA Chemistry Data Series will encourage other authors to publish their own collections of thermophysical data and it goes without saying that we would be happy to pass on the experience we have accumulated over the years.

Finally, no new edition would be complete without a word of thanks to our readers – scientists and engineers from the thermophysical data community – for their constructive suggestions and input which have contributed to its success. We are confident that you will find this new edition of the DECHEMA Chemistry Data Series not only useful, but also interesting and inspiring.

Frankfurt am Main, December 2012

Richard Sass

CONTENTS
Vol. I, Part 4

In Part 4c:

Subjects of Chemistry Data Series Vol. I	vi
Author's Preface	vii
Executive Editor's Preface	viii
Contents Vol. I, Part 4c	ix
Guide to Tables	xi
References	xxiii

Data Tables

Binary Systems	1
Ternary Systems	550
Quaternary Systems	573
Appendix A: Pure Component Parameters	575
Appendix B: Dimerization Constants of Carboxylic Acids	583
Formula Index of Binary Systems	587
Alphabetical Index of Binary Systems	594
Formula Index of Ternary Systems	602
Alphabetical Index of Ternary Systems	603
Formula Index of Quaternary Systems	604
Alphabetical Index of Quaternary Systems	605

Part 4c contains pages i–xxiii and 1–605.

Ethers

Formula Index of Binary Systems

C ₂ H ₄ O	Ethylene oxide	C ₄ H ₁₀ O ₃	Diethylene glycol	2, 3
		C ₈ H ₁₈ O ₅	Tetraethylene glycol	4, 5
C ₂ H ₆ O	Dimethyl ether	C ₃ H ₆ O ₂	Formic acid ethyl ester	6
C ₃ H ₅ ClO	Epichlorohydrin	C ₂ H ₆ OS	Dimethyl sulfoxide	7–9
		C ₃ H ₄ Cl ₂	2,3-Dichloropropene	10
		C ₃ H ₆ Cl ₂ O	1,3-Dichloro-2-propanol	11, 12
		C ₃ H ₆ Cl ₂ O	2,3-Dichloro-1-propanol	13
		C ₃ H ₇ ClO ₂	3-Chloro-1,2-propanediol	14, 15
		C ₆ H ₁₂	Cyclohexane	16
		C ₆ H ₁₄ O ₃	Diethylene glycol dimethyl ether	17
		C ₇ H ₈	Toluene	18–23
		C ₈ H ₁₀	Ethylbenzene	24
		C ₈ H ₁₀	m-Xylene	25–27
		C ₁₀ H ₂₂	Decane	28
C ₃ H ₆ O	1,2-Propylene oxide	C ₃ H ₅ Cl	cis-1-Chloropropene	29, 30
		C ₃ H ₅ Cl	trans-1-Chloropropene	31, 32
		C ₆ H ₁₄	2-Methylpentane	33, 34
C ₃ H ₆ O ₂	1,3-Dioxolane	C ₃ H ₇ Cl	1-Chloropropane	35–37
		C ₄ H ₉ Cl	Butyl chloride	38–44
		C ₄ H ₉ Cl	sec-Butyl chloride	45–51
		C ₄ H ₉ Cl	tert-Butyl chloride	52–56
		C ₄ H ₉ Cl	1-Chloro-2-methylpropane	57–61
		C ₄ H ₉ Cl	Butyl chloride	62
		C ₅ H ₁₀	Cyclopentane	63–65
		C ₅ H ₁₀ O ₃	Carbonic acid diethyl ester	66
		C ₅ H ₁₁ Cl	1-Chloropentane	67–72
		C ₅ H ₁₂ O	Methyl tert-butyl ether (MTBE)	73
		C ₆ H ₆	Benzene	74–77
		C ₆ H ₇ N	Aniline	78
		C ₆ H ₁₂	Cyclohexane	79–84
		C ₆ H ₁₃ Cl	1-Chlorohexane	85–89
		C ₆ H ₁₄	Hexane	90–92
		C ₇ H ₁₆	Heptane	93
C ₈ H ₁₈	2,2,4-Trimethylpentane	94		
C ₃ H ₆ O ₂	2,3-Epoxy-1-propanol	C ₄ H ₁₀ O ₂	1-Methoxy-2-propanol	95, 96

C ₃ H ₆ O ₃	1,3,5-Trioxane	C ₂ H ₄ Cl ₂	1,2-Dichloroethane	97
		C ₆ H ₆	Benzene	98
		C ₆ H ₁₂	Cyclohexane	99
C ₃ H ₈ O ₂	Dimethoxymethane	C ₅ H ₁₂ O	Methyl tert-butyl ether (MTBE)	100
		C ₆ H ₆	Benzene	101, 102
		C ₆ H ₁₂	Cyclohexane	103, 104
		C ₆ H ₁₄	Hexane	105
		C ₆ H ₁₄ O	Diisopropyl ether	106
		C ₇ H ₈	Toluene	107
		C ₈ H ₁₈	2,2,4-Trimethylpentane	108
C ₃ H ₈ O ₂	2-Methoxyethanol	C ₂ HCl ₃	Trichloroethylene	109–111
		C ₃ H ₆ O ₂	Methyl acetate	112
		C ₄ H ₈ O	Tetrahydrofuran	113
		C ₄ H ₁₁ NO	N,N-Dimethylethanolamine	114, 115
		C ₆ H ₁₀	Cyclohexene	116
		C ₆ H ₁₂	Cyclohexane	117–121
		C ₆ H ₁₄	Hexane	122, 123
		C ₆ H ₁₄ O	Diisopropyl ether	124–127
		C ₇ H ₁₆	Heptane	128
C ₈ H ₁₀	o-Xylene	129, 130		
C ₄ H ₄ F ₆ O	bis(2,2,2-Trifluoroethyl)ether [HFE356MF-F]	C ₄ H ₈ O ₂	Ethyl acetate	131
		C ₆ H ₁₄ O	Ethyl butyl ether	132
C ₄ H ₄ O	Furan	C ₅ H ₆ O	2-Methylfuran	133
C ₄ H ₆ O	2,3-Dihydrofuran	C ₄ H ₈ O	Tetrahydrofuran	134, 135
C ₄ H ₈ Cl ₂ O	bis(2-Chloroethyl) ether	C ₆ H ₁₂ Cl ₂ O ₂	1,8-Dichloro-3,6-Dioxaoctane	136
C ₄ H ₈ O	2,2-Dimethyloxirane	C ₄ H ₈ O	1,2-Epoxybutane	137, 138
C ₄ H ₈ O	1,2-Epoxybutane	CHCl ₃	Chloroform	139–142
		C ₃ H ₆ O ₂	Methyl acetate	143–146
		C ₃ H ₆ O ₃	Carbonic acid dimethyl ester	147, 148
C ₄ H ₈ O	2-Methoxypropene	C ₅ H ₁₂ O ₂	2,2-Dimethoxypropane	149

C ₄ H ₈ O	Tetrahydrofuran	CCl ₄	Tetrachloromethane	150
		CHCl ₃	Chloroform	151–154
		C ₂ Cl ₄	Tetrachloroethylene	155–162
		C ₂ HCl ₃	Trichloroethylene	163
		C ₂ H ₂ Cl ₄	1,1,2,2-Tetrachloroethane	164–172
		C ₂ H ₃ Cl ₃	1,1,1-Trichloroethane (R140A)	173
		C ₂ H ₃ N	Acetonitrile	174, 175
		C ₂ H ₄ Cl ₂	1,2-Dichloroethane	176
		C ₃ H ₆ O ₂	Methyl acetate	177
		C ₃ H ₇ Cl	1-Chloropropane	178–183
		C ₄ H ₆ O ₂	Vinyl acetate	184
		C ₄ H ₈ O ₂ S	Sulfolane	185
		C ₄ H ₉ Cl	Butyl chloride	186, 187
		C ₄ H ₉ Cl	sec-Butyl chloride	188, 189
		C ₄ H ₉ Cl	tert-Butyl chloride	190
		C ₄ H ₉ Cl	1-Chloro-2-methylpropane	191, 192
		C ₅ H ₆ O	2-Methylfuran	193, 194
		C ₅ H ₁₀	2-Methyl-2-butene	195, 196
		C ₅ H ₁₁ Cl	1-Chloropentane	197–201
		C ₅ H ₁₂	Pentane	202–207
		C ₅ H ₁₂ O	Methyl tert-butyl ether (MTBE)	208
		C ₆ H ₅ Br	Bromobenzene	209, 210
		C ₆ H ₅ Cl	Chlorobenzene	211–213
		C ₆ H ₁₁ Br	Bromocyclohexane	214–216
		C ₆ H ₁₁ Cl	Chlorocyclohexane	217, 218
		C ₆ H ₁₂	Cyclohexane	219, 220
		C ₆ H ₁₃ Cl	1-Chlorohexane	221
		C ₆ H ₁₄	Hexane	222–228
		C ₆ H ₁₄	3-Methylpentane	229
		C ₆ H ₁₄ O	Ethyl tert-butyl ether (ETBE)	230–232
		C ₆ H ₁₄ O	Methyl tert-amyl ether (TAME)	233, 234
		C ₆ H ₁₈ OSi ₂	Hexamethyl disiloxane	235
		C ₇ H ₈	Toluene	236, 237
		C ₇ H ₁₄	Methylcyclohexane	238
		C ₇ H ₁₆	Heptane	239–249
		C ₈ H ₁₀	p-Xylene	250

C ₄ H ₈ O	Tetrahydrofuran	C ₈ H ₁₈	Octane	251
		C ₈ H ₁₈	2,2,4-Trimethylpentane	252, 253
		C ₈ H ₁₈ O	Dibutyl ether	254
		C ₉ H ₁₂	Isopropylbenzene	255
		C ₁₀ H ₂₂	Decane	256
C ₄ H ₈ O ₂	1,4-Dioxane	Cl ₄ Si	Tetrachlorosilane	257
		O ₂ S	Sulfur dioxide	258
		C ₂ H ₆ OS	Dimethyl sulfoxide	259–264
		C ₃ H ₇ Cl	1-Chloropropane	265
		C ₄ H ₈ O ₂ S	Sulfolane	266
		C ₄ H ₉ Cl	Butyl chloride	267–272
		C ₄ H ₉ Cl	sec-Butyl chloride	273–278
		C ₄ H ₉ Cl	tert-Butyl chloride	279–284
		C ₄ H ₉ Cl	1-Chloro-2-methylpropane	285–289
		C ₅ H ₁₀	Cyclopentane	290–293
		C ₅ H ₁₁ Cl	1-Chloropentane	294–299
		C ₆ H ₆	Benzene	300–303
		C ₆ H ₁₂	Cyclohexane	304–311
		C ₆ H ₁₃ Cl	1-Chlorohexane	312–315
		C ₆ H ₁₄	Hexane	316
		C ₆ H ₁₈ OSi ₂	Hexamethyl disiloxane	317
		C ₇ H ₉ N	N-Methylaniline	318
C ₇ H ₉ N	o-Methylaniline	319		
C ₄ H ₁₀ O	Diethyl ether	CS ₂	Carbon disulfide	320–322
		CHBr ₃	Tribromomethane [R20B3]	323, 324
		CHCl ₃	Chloroform	325, 326
		C ₂ HCl ₅	Pentachloroethane	327
		C ₂ H ₃ Cl ₃	1,1,1-Trichloroethane [R140A]	328
		C ₄ H ₅ NS	Allyl isothiocyanate	329
		C ₆ F ₁₄	Perfluorohexane	330
		C ₆ H ₅ NO ₂	Nitrobenzene	331, 332
		C ₆ H ₆	Benzene	333
		C ₆ H ₇ N	Aniline	334
		C ₆ H ₁₄ O	Ethyl tert-butyl ether (ETBE)	335–338
		C ₆ H ₁₅ N	Triethylamine	339

C ₄ H ₁₀ O	Diethyl ether	C ₇ H ₈ O	Methoxybenzene	340, 341
		C ₇ H ₈ O ₂	2-Methoxyphenol	342
		C ₈ H ₁₈ O	Dibutyl ether	343
		C ₁₀ H ₁₂	1,2,3,4-Tetrahydronaphthalene	344
		C ₁₀ H ₁₈	Decalin <isomer not specified>	345
C ₄ H ₁₀ O ₂	1,2-Dimethoxyethane	C ₆ H ₁₂	Cyclohexane	346
		C ₁₀ H ₂₂	Decane	347
C ₄ H ₁₀ O ₂	2-Ethoxyethanol	CCl ₄	Tetrachloromethane	348
		CH ₂ Cl ₂	Dichloromethane	349
		C ₂ H ₄ Cl ₂	1,2-Dichloroethane	350
		C ₂ H ₄ O ₂	Methyl formate	351
		C ₃ H ₆ O ₂	Methyl acetate	352, 353
		C ₃ H ₆ O ₃	Carbonic acid dimethyl ester	354–356
		C ₄ H ₈ O ₂	Ethyl acetate	357, 358
		C ₅ H ₁₀ O ₂	Acetic acid propyl ester	359
		C ₅ H ₁₀ O ₂	Formic acid butyl ester	360, 361
		C ₅ H ₁₀ O ₂	Propanoic acid ethyl ester	362
		C ₆ H ₁₂	Cyclohexane	363–365
		C ₆ H ₁₄	Hexane	366, 367
		C ₆ H ₁₄ O	di-n-Propyl ether	368–371
		C ₇ H ₁₂ O ₃	Ethoxy ethyl acrylate	372
		C ₇ H ₁₆	Heptane	373, 374
		C ₈ H ₁₀	o-Xylene	375
		C ₈ H ₁₆	2,4,4-Trimethyl-1-pentene	376
C ₈ H ₁₈	Octane	377		
C ₄ H ₁₀ O ₂	1-Methoxy-2-propanol	C ₅ H ₁₃ N	1-Aminopentane	378–380
		C ₆ H ₁₄ O	Diisopropyl ether	381–383
C ₄ H ₁₀ O ₂	Propylene glycol monomethyl ether	C ₂ H ₄ O ₂	Acetic acid	384
		C ₂ H ₅ NO ₂	Nitroethane	385, 386
		C ₆ H ₁₂ O ₃	Propylene glycol monomethyl ether acetate	387–390
C ₄ H ₁₀ O ₃	Diethylene glycol	C ₂ H ₆ OS	Dimethyl sulfoxide	391
		C ₂ H ₇ NO	Monoethanolamine	392
		C ₇ H ₈ O ₂	2-Methoxyphenol	393–396

C ₅ H ₆ O	2-Methylfuran	C ₇ H ₁₆	Heptane	397
C ₅ H ₆ O ₂	Furfuryl alcohol	C ₅ H ₁₀ O ₂	Tetrahydrofurfuryl alcohol	398–400
C ₅ H ₈ O ₂	Tetrahydropyran-2-one	C ₆ H ₆	Benzene	401–403
C ₅ H ₁₀ O	2-Methyltetrahydrofuran	C ₆ H ₅ Br	Bromobenzene	404, 405
		C ₆ H ₅ Cl	Chlorobenzene	406, 407
		C ₆ H ₁₁ Br	Bromocyclohexane	408, 409
		C ₆ H ₁₁ Cl	Chlorocyclohexane	410, 411
		C ₆ H ₁₂	Cyclohexane	412, 413
		C ₇ H ₈	Toluene	414, 415
		C ₇ H ₁₄	Methylcyclohexane	416
		C ₈ H ₁₈	2,2,4-Trimethylpentane	417, 418
		C ₉ H ₁₂	Isopropylbenzene	419
C ₅ H ₁₀ O	Tetrahydropyran	CHCl ₃	Chloroform	420
		C ₃ H ₇ Cl	1-Chloropropane	421–425
		C ₄ H ₉ Cl	Butyl chloride	426, 427
		C ₄ H ₉ Cl	sec-Butyl chloride	428–430
		C ₄ H ₉ Cl	tert-Butyl chloride	431
		C ₄ H ₉ Cl	1-Chloro-2-methylpropane	432, 433
		C ₅ H ₁₁ Cl	1-Chloropentane	434–438
		C ₆ H ₅ Br	Bromobenzene	439, 440
		C ₆ H ₅ Cl	Chlorobenzene	441, 442
		C ₆ H ₇ N	Aniline	443
		C ₆ H ₁₁ Br	Bromocyclohexane	444, 445
		C ₆ H ₁₁ Cl	Chlorocyclohexane	446–448
		C ₆ H ₁₂	Cyclohexane	449
		C ₆ H ₁₃ Cl	1-Chlorohexane	450–452
		C ₆ H ₁₄	Hexane	453–456
		C ₇ H ₈	Toluene	457–462
		C ₇ H ₉ N	N-Methylaniline	463
		C ₇ H ₉ N	o-Methylaniline	464
		C ₇ H ₁₄	Cycloheptane	465
		C ₇ H ₁₆	Heptane	466–471
		C ₈ H ₁₆	Cyclooctane	472
		C ₈ H ₁₈	2,2,4-Trimethylpentane	473
		C ₉ H ₁₂	Isopropylbenzene	474

C ₅ H ₁₂ O	Methyl butyl ether	C ₆ F ₁₄	Perfluorohexane	475, 476
		C ₆ H ₁₀	2-Hexyne	477–480
C ₅ H ₁₂ O	Methyl tert-butyl ether (MTBE)	CHCl ₃	Chloroform	481–483
		C ₂ H ₃ N	Acetonitrile	484
		C ₄ H ₉ Cl	Butyl chloride	485–487
		C ₄ H ₉ Cl	sec-Butyl chloride	488–491
		C ₄ H ₉ Cl	tert-Butyl chloride	492–495
		C ₄ H ₉ Cl	1-Chloro-2-methylpropane	496–499
		C ₅ H ₁₀	2-Methyl-1-butene	500
		C ₆ H ₆	Benzene	501–503
		C ₆ H ₁₀	1-Hexyne	504–513
		C ₆ H ₁₀	2-Hexyne	514–516
		C ₆ H ₁₂	Cyclohexane	517–522
		C ₆ H ₁₂	1-Hexene	523, 524
		C ₆ H ₁₄	Hexane	525
		C ₆ H ₁₄	2-Methylpentane	526
		C ₆ H ₁₄	3-Methylpentane	527
		C ₇ H ₈	Toluene	528–532
		C ₇ H ₁₄	Methylcyclohexane	533
		C ₇ H ₁₆	Heptane	534–537
		C ₈ H ₁₈	Octane	538, 539
		C ₈ H ₁₈	2,2,4-Trimethylpentane	540–546
C ₁₀ H ₂₂	Decane	547–549		

bis(2-Chloroethyl) ether	$C_4H_8Cl_2O$	1,8-Dichloro-3,6-Dioxaoctane	$C_6H_{12}Cl_2O_2$	136
bis(2,2,2-Trifluoroethyl) ether [HFE356MF-F]	$C_4H_4F_6O$	Ethyl acetate	$C_4H_8O_2$	131
Dibutyl ether	$C_8H_{18}O$	Diethyl ether	$C_4H_{10}O$	343
		Tetrahydrofuran	C_4H_8O	254
Diethylene glycol	$C_4H_{10}O_3$	Ethylene oxide	C_2H_4O	2, 3
		Dimethyl sulfoxide	C_2H_6OS	391
		2-Methoxyphenol	$C_7H_8O_2$	393–396
		Monoethanolamine	C_2H_7NO	392
Diethylene glycol dimethyl ether	$C_6H_{14}O_3$	Epichlorohydrin	C_3H_5ClO	17
Diethyl ether	$C_4H_{10}O$	Allyl isothiocyanate	C_4H_5NS	329
		Aniline	C_6H_7N	334
		Benzene	C_6H_6	333
		Carbon disulfide	CS_2	320–322
		Chloroform	$CHCl_3$	325, 326
		Decalin isomer not specified	$C_{10}H_{18}$	345
		Ethyl tert-butyl ether (ETBE)	$C_6H_{14}O$	335–338
		Methoxybenzene	C_7H_8O	340, 341
		2-Methoxyphenol	$C_7H_8O_2$	342
		Nitrobenzene	$C_6H_5NO_2$	331, 332
		Pentachloroethane	C_2HCl_5	327
		Perfluorohexane	C_6F_{14}	330
		1,2,3,4-Tetrahydro- naphthalene	$C_{10}H_{12}$	344
		Tribromomethane [R20B3]	$CHBr_3$	323, 324
		1,1,1-Trichloroethane [R140A]	$C_2H_3Cl_3$	328
		Triethylamine	$C_6H_{15}N$	339
2,3-Dihydrofuran	C_4H_6O	Tetrahydrofuran	C_4H_8O	134, 135
Diisopropyl ether	$C_6H_{14}O$	Dimethoxymethane	$C_3H_8O_2$	106
		2-Methoxyethanol	$C_3H_8O_2$	124–127
		1-Methoxy- 2-propanol	$C_4H_{10}O_2$	381–383

Ethers

Alphabetical Index of Binary Systems

1,2-Dimethoxyethane	C ₄ H ₁₀ O ₂	Cyclohexene	C ₆ H ₁₂	346
		Decane	C ₁₀ H ₂₂	347
Dimethoxymethane	C ₃ H ₈ O ₂	Benzene	C ₆ H ₆	101, 102
		Cyclohexane	C ₆ H ₁₀	103, 104
		Hexane	C ₆ H ₁₄	105
		Methyl tert-butyl ether (MTBE)	C ₅ H ₁₂ O	100
		Toluene	C ₇ H ₈	107
		2,2,4-Trimethylpentane	C ₈ H ₁₈	108
2,2-Dimethoxypropane	C ₅ H ₁₂ O ₂	2-Methoxypropene	C ₄ H ₈ O	149
Dimethyl ether	C ₂ H ₆ O	Formic acid ethyl ester	C ₃ H ₆ O ₂	6
2,2-Dimethyloxirane	C ₄ H ₈ O	1,2-Epoxybutane	C ₄ H ₈ O	137, 138
1,4-Dioxane	C ₄ H ₈ O ₂	Benzene	C ₆ H ₆	300–303
		Butyl chloride	C ₄ H ₉ Cl	267–272
		sec-Butyl chloride	C ₄ H ₉ Cl	273–278
		tert-Butyl chloride	C ₄ H ₉ Cl	279–284
		1-Chlorohexane	C ₆ H ₁₃ Cl	312–315
		1-Chloro-2-methylpropane	C ₄ H ₉ Cl	285–289
		1-Chloropentane	C ₅ H ₁₁ Cl	294–299
		1-Chloropropane	C ₃ H ₇ Cl	265
		Cyclohexane	C ₆ H ₁₀	304–311
		Cyclopentane	C ₅ H ₁₀	290–293
		Dimethyl sulfoxide	C ₂ H ₆ OS	259–264
		Hexamethyl disiloxane	C ₆ H ₁₈ OSi ₂	317
		Hexane	C ₆ H ₁₄	316
		N-Methylaniline	C ₇ H ₉ N	318
		o-Methylaniline	C ₇ H ₉ N	319
		Sulfolane	C ₄ H ₈ O ₂ S	266
		Sulfur dioxide	O ₂ S	258
Tetrachlorosilane	Cl ₄ Si	257		

1,3-Dioxolane	$C_3H_6O_2$	Aniline	C_6H_7N	78
		Benzene	C_6H_6	74–77
		Butyl chloride	C_4H_9Cl	38–44, 62
		sec-Butyl chloride	C_4H_9Cl	45–51
		tert-Butyl chloride	C_4H_9Cl	52–56
		Carbonic acid diethyl ester	$C_5H_{10}O_3$	66
		1-Chlorohexane	$C_6H_{13}Cl$	85–89
		1-Chloro-2-methylpropane	C_4H_9Cl	57–61
		1-Chloropentane	$C_5H_{11}Cl$	67–72
		1-Chloropropane	C_3H_7Cl	35–37
		Cyclohexane	C_6H_{10}	79–84
		Cyclopentane	C_5H_{10}	63–65
		Heptane	C_7H_{16}	93
		Hexane	C_6H_{14}	90–92
		Methyl tert-butyl ether (MTBE)	$C_5H_{12}O$	73
		2,2,4-Trimethylpentane	C_8H_{18}	94
		Epichlorohydrin	C_3H_5ClO	3-Chloro-1,2-propanediol
Cyclohexane	C_6H_{10}			16
Decane	$C_{10}H_{22}$			28
1,3-Dichloro-2-propanol	$C_3H_6Cl_2O$			11, 12
2,3-Dichloro-1-propanol	$C_3H_6Cl_2O$			13
2,3-Dichloropropene	$C_3H_4Cl_2$			10
Dimethyl sulfoxide	C_2H_6OS			7–9
Ethylbenzene	C_8H_{10}			24
Toluene	C_7H_8			18–23
m-Xylene	C_8H_{10}			25–27
1,2-Epoxybutane	C_4H_8O			Carbonic acid dimethyl ester
		Chloroform	$CHCl_3$	139–142
		Methyl acetate	$C_3H_6O_2$	143–146

2,3-Epoxy-1-propanol	$C_3H_6O_2$	1-Methoxy-2-propanol	$C_4H_{10}O_2$	95, 96
2-Ethoxyethanol	$C_4H_{10}O_2$	Acetic acid propyl ester	$C_5H_{10}O_2$	359
		Carbonic acid dimethyl ester	$C_3H_6O_3$	354–356
		Cyclohexane	C_6H_{10}	363–365
		1,2-Dichloroethane	$C_2H_4Cl_2$	350
		Dichloromethane	CH_2Cl_2	349
		Ethoxy ethyl acrylate	$C_7H_{12}O_3$	372
		Ethyl acetate	$C_4H_8O_2$	357, 358
		Formic acid butyl ester	$C_5H_{10}O_2$	360, 361
		Heptane	C_7H_{16}	373, 374
		Hexane	C_6H_{14}	366, 367
		Methyl acetate	$C_3H_6O_2$	352, 353
		Methyl formate	$C_2H_4O_2$	351
		Octane	C_8H_{18}	377
		Propanoic acid ethyl ester	$C_5H_{10}O_2$	362
		di-n-Propyl ether	$C_6H_{14}O$	368–371
		Tetrachloromethane	CCl_4	348
		2,4,4-Trimethyl-1-pentene	C_8H_{16}	376
		o-Xylene	C_8H_{10}	375
Ethyl butyl ether	$C_6H_{14}O$	bis(2,2,2-Trifluoroethyl) ether [HFE356MF-F]	$C_4H_4F_6O$	132
Ethyl tert-butyl ether (ETBE)	$C_6H_{14}O$	Tetrahydrofuran	C_4H_8O	230–232
Ethylene oxide	C_2H_4O	Tetraethylene glycol	$C_8H_{18}O_5$	4, 5
Furan	C_4H_4O	2-Methylfuran	C_5H_6O	133
Furfuryl alcohol	$C_5H_6O_2$	Tetrahydrofurfuryl alcohol	$C_5H_{10}O_2$	398–400
2-Methoxyethanol	$C_3H_8O_2$	Cyclohexane	C_6H_{10}	116–121
		N,N-Dimethyl-ethanolamine	$C_4H_{11}NO$	114, 115
		Heptane	C_7H_{16}	128

2-Methoxyethanol	$C_3H_8O_2$	Hexane	C_6H_{14}	122, 123
		Methyl acetate	$C_3H_6O_2$	112
		Tetrahydrofuran	C_4H_8O	113
		Trichloroethylene	C_2HCl_3	109–111
		o-Xylene	C_8H_{10}	129, 130
1-Methoxy-2-propanol	$C_4H_{10}O_2$	1-Aminopentane	$C_5H_{13}N$	378–380
Methyl butyl ether	$C_5H_{12}O$	2-Hexyne	C_6H_{10}	477–480
		Perfluorohexane	C_6F_{14}	475, 476
2-Methylfuran	C_5H_6O	Heptane	C_7H_{16}	397
		Tetrahydrofuran	C_4H_8O	193, 194
Methyl tert-amyl ether (TAME)	$C_6H_{14}O$	Tetrahydrofuran	C_4H_8O	233, 234
Methyl tert-butyl ether (MTBE)	$C_5H_{12}O$	Acetonitrile	C_2H_3N	484
		Benzene	C_6H_6	501–503
		Butyl chloride	C_4H_9Cl	485–487
		sec-Butyl chloride	C_4H_9Cl	488–491
		tert-Butyl chloride	C_4H_9Cl	492–495
		Chloroform	$CHCl_3$	481–483
		1-Chloro-2-methylpropane	C_4H_9Cl	496–499
		Cyclohexane	C_6H_{10}	517–522
		Decane	$C_{10}H_{22}$	547–549
		Heptane	C_7H_{16}	534–537
		Hexane	C_6H_{14}	525
		1-Hexene	C_6H_{12}	523, 524
		1-Hexyne	C_6H_{10}	504–513
		2-Hexyne	C_6H_{10}	514–516
		2-Methyl-1-butene	C_5H_{10}	500
		Methylcyclohexane	C_7H_{14}	533
		2-Methylpentane	C_6H_{14}	526
		3-Methylpentane	C_6H_{14}	527
		Octane	C_8H_{18}	538, 539
		Tetrahydrofuran	C_4H_8O	208
		Toluene	C_7H_8	528–532
		2,2,4-Trimethylpentane	C_8H_{18}	540–546

Ethers

Alphabetical Index of Binary Systems

2-Methyltetrahydrofuran	C ₅ H ₁₀ O	Bromobenzene	C ₆ H ₅ Br	404, 405
		Bromocyclohexane	C ₆ H ₁₁ Br	408, 409
		Chlorobenzene	C ₆ H ₅ Cl	406, 407
		Chlorocyclohexane	C ₆ H ₁₁ Cl	410, 411
		Cyclohexane	C ₆ H ₁₀	412, 413
		Isopropylbenzene	C ₉ H ₁₂	419
		Methylcyclohexane	C ₇ H ₁₄	416
		Toluene	C ₇ H ₈	414, 415
		2,2,4-Trimethylpentane	C ₈ H ₁₈	417, 418
Propylene glycol monomethyl ether	C ₄ H ₁₀ O ₂	Acetic acid	C ₂ H ₄ O ₂	384
		Nitroethane	C ₂ H ₅ NO ₂	385, 386
		Propylene glycol monomethyl ether acetate	C ₆ H ₁₂ O ₃	387–390
1,2-Propylene oxide	C ₃ H ₆ O	cis-1-Chloropropene	C ₃ H ₅ Cl	29, 30
		trans-1-Chloropropene	C ₃ H ₅ Cl	31, 32
		2-Methylpentane	C ₆ H ₁₄	33, 34
Tetrahydrofuran	C ₄ H ₈ O	Acetonitrile	C ₂ H ₃ N	174, 175
		Bromobenzene	C ₆ H ₅ Br	209, 210
		Bromocyclohexane	C ₆ H ₁₁ Br	214–216
		Butyl chloride	C ₄ H ₉ Cl	186, 187
		sec-Butyl chloride	C ₄ H ₉ Cl	188, 189
		tert-Butyl chloride	C ₄ H ₉ Cl	190
		Chlorobenzene	C ₆ H ₅ Cl	211–213
		Chlorocyclohexane	C ₆ H ₁₁ Cl	217, 218
		Chloroform	CHCl ₃	151–154
		1-Chlorohexane	C ₆ H ₁₃ Cl	221
		1-Chloro-2-methylpropane	C ₄ H ₉ Cl	191, 192
		1-Chloropentane	C ₅ H ₁₁ Cl	197–201
		1-Chloropropane	C ₃ H ₇ Cl	178–183
		Cyclohexane	C ₆ H ₁₀	219, 220
		Decane	C ₁₀ H ₂₂	256
		1,2-Dichloroethane	C ₂ H ₄ Cl ₂	176

Tetrahydrofuran	C_4H_8O	Heptane	C_7H_{16}	239–249
		Hexamethyl disiloxane	$C_6H_{18}OSi_2$	235
		Hexane	C_6H_{14}	222–228
		Isopropylbenzene	C_9H_{12}	255
		Methyl acetate	$C_3H_6O_2$	177
		2-Methyl-2-butene	C_5H_{10}	195, 196
		Methylcyclohexane	C_7H_{14}	238
		3-Methylpentane	C_6H_{14}	229
		Octane	C_8H_{18}	251
		Pentane	C_5H_{12}	202–207
		Sulfolane	$C_4H_8O_2S$	185
		1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	164–172
		Tetrachloroethylene	C_2Cl_4	155–162
		Tetrachloromethane	CCl_4	150
		Toluene	C_7H_8	236, 237
		1,1,1-Trichloroethane [R140A]	$C_2H_3Cl_3$	173
		Trichloroethylene	C_2HCl_3	163
		2,2,4-Trimethylpentane	C_8H_{18}	252, 253
		Vinyl acetate	$C_4H_6O_2$	184
		p-Xylene	C_8H_{10}	250
Tetrahydropyran	$C_5H_{10}O$	Aniline	C_6H_7N	443
		Bromobenzene	C_6H_5Br	439, 440
		Bromocyclohexane	$C_6H_{11}Br$	444, 445
		Butyl chloride	C_4H_9Cl	426, 427
		sec-Butyl chloride	C_4H_9Cl	428–430
		tert-Butyl chloride	C_4H_9Cl	431
		Chlorobenzene	C_6H_5Cl	441, 442
		Chlorocyclohexane	$C_6H_{11}Cl$	446–448
		Chloroform	$CHCl_3$	420
		1-Chlorohexane	$C_6H_{13}Cl$	450–452
		1-Chloro-2-methylpropane	C_4H_9Cl	432, 433

Ethers

Alphabetical Index of Binary Systems

Tetrahydropyran	$C_5H_{10}O$	1-Chloropentane	$C_5H_{11}Cl$	434–438
		1-Chloropropane	C_3H_7Cl	421–425
		Cycloheptane	C_7H_{14}	465
		Cyclohexane	C_6H_{10}	449
		Cyclooctane	C_8H_{16}	472
		Heptane	C_7H_{16}	466–471
		Hexane	C_6H_{14}	453–456
		Isopropylbenzene	C_9H_{12}	474
		N-Methylaniline	C_7H_9N	463
		o-Methylaniline	C_7H_9N	464
		Toluene	C_7H_8	457–462
		2,2,4-Trimethyl- pentane	C_8H_{18}	473
Tetrahydropyran-2-one	$C_5H_8O_2$	Benzene	C_6H_6	401–403
1,3,5-Trioxane	$C_3H_6O_3$	Benzene	C_6H_6	98
		Cyclohexane	C_6H_{10}	99
		1,2-Dichloroethane	$C_2H_4Cl_2$	97

C_3H_5ClO	Epichlorohydrin	$C_4H_8O_2$	1,4-Dioxane	$C_6H_{14}O_3$	Diethylene glycol dimethyl ether	550
$C_3H_8O_2$	2-Methoxyethanol	C_4H_8O	Tetrahydrofuran	C_6H_{12}	Cyclohexane	551, 552
		C_6H_{10}	Cyclohexene	C_6H_{12}	Cyclohexane	553, 554
C_4H_8O	Tetrahydrofuran	$CHCl_3$	Chloroform	C_6H_{12}	Cyclohexane	555, 556
		$C_4H_8O_2$	Ethyl acetate	C_6H_{12}	Cyclohexane	557
		$C_5H_2F_{10}$	1,1,1,2,3,4,4,5,5- Decafluoropentane [R43-10MEE]	C_5H_6O	2-Methylfuran	558, 559
		$C_5H_{12}O$	Methyl tert-butyl ether (MTBE)	C_7H_{16}	Heptane	560, 561
$C_4H_{10}O_2$	2-Ethoxyethanol	$C_6H_{12}O_2$	Acetic acid butyl ester	C_7H_8	Toluene	562
$C_4H_{10}O_3$	Diethylene glycol	$C_6H_{14}O_2$	2-Butoxyethanol	$C_8H_{18}O_3$	Diethylene glycol monobutyl ether	563
$C_5H_{12}O$	Methyl tert-butyl ether (MTBE)	C_6H_6	Benzene	C_6H_{12}	1-Hexene	564
				C_7H_8	Toluene	565
				C_7H_{16}	Heptane	566
		C_6H_{12}	Cyclohexane	C_6H_{12}	1-Hexene	567
				C_7H_{16}	Heptane	568
		C_6H_{12}	1-Hexene	C_7H_{16}	Heptane	569, 570
		C_7H_{16}	Heptane	C_8H_{18}	Octane	571, 572

Ethers

Alphabetical Index of Ternary Systems

2-Butoxyethanol	$C_6H_{14}O_2$	Diethylene glycol	$C_4H_{10}O_3$	Diethylene glycol monobutyl ether	$C_8H_{18}O_3$	563
Diethylene glycol dimethyl ether	$C_6H_{14}O_3$	1,4-Dioxane	$C_4H_8O_2$	Epichlorohydrin	C_3H_5ClO	550
2-Ethoxyethanol	$C_4H_{10}O_2$	Acetic acid butyl ester	$C_6H_{12}O_2$	Toluene	C_7H_8	562
2-Methoxyethanol	$C_3H_8O_2$	Cyclohexane	C_6H_{12}	Cyclohexene	C_6H_{10}	553, 554
				Tetrahydrofuran	C_4H_8O	551, 552
Methyl tert-butyl ether (MTBE)	$C_5H_{12}O$	Benzene	C_6H_6	Heptane	C_7H_{16}	566
				1-Hexene	C_6H_{12}	564
				Toluene	C_7H_8	565
		Cyclohexane	C_6H_{12}	1-Hexene	C_6H_{12}	567
				Heptane	C_7H_{16}	568
		Heptane	C_7H_{16}	1-Hexene	C_6H_{12}	569, 570
				Octane	C_8H_{18}	571, 572
				Tetrahydrofuran	C_4H_8O	560, 561
2-Methylfuran	C_5H_6O	1,1,1,2,3,4,4,5,5,5-Decafluoropentane [R43-10MEE]	$C_5H_2F_{10}$	Tetrahydrofuran	C_4H_8O	558, 559
Tetrahydrofuran	C_4H_8O	Chloroform	$CHCl_3$	Cyclohexane	C_6H_{12}	555, 556
		Cyclohexane	C_6H_{12}	Ethyl acetate	$C_4H_8O_2$	557

$C_4H_{10}O_2$	2-Ethoxyethanol	C_8H_8	Styrene	C_8H_{10}	m-Xylene	C_8H_{10}	p-Xylene	573
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Ethers**Alphabetical Index of Quaternary Systems**

2-Ethoxyethanol	$C_4H_{10}O_2$	Styrene	C_8H_8	m-Xylene	C_8H_{10}	p-Xylene	C_8H_{10}	573
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