水道水及び水道原水中の微量有機化合物の一覧表

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[平成8年6月3日受理]

Trace Organic Compounds in Tap Water and Raw Water

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[Received June 3, 1996]

Summary

A list of trace organic compounds found in tap water and raw water was prepared from lists of organic compounds in effluent from pulp mill, environmental water and our unpublished data.

The list does not contain perfumeries, polyaromatic compounds, organometallic compounds, dioxins and related compounds, organophosphoric acid triesters, phthalic acid esters, adipitic acid esters, insecticides and herbicides of medium and high boiling points.

Key words: organic compound, tap water, raw water, chlorination, disinfectant by-product

1. はじめに

特に、北欧のダイオキシン研究者は塩素漂白処理を施したパルプ工場排水中の微量有機物の同定確認を精力的に行ってきた。また欧米の水道水専門家等はそのデータを活用し、水道水中の消毒副生成物の同定確認を行っている。その結果として、トリハロメタン以外の極一部の消毒副生成物は世界保健機関 (WHO)、米国環境保護庁 (EPA) の飲料水の水質基準、及び日本の水道水質基準の監視項目に設定された。

その為現在日本では、それら消毒副生成物等が頻繁に測定されるようになってきている。そして、ガスクロマトグラム上に未知ピークが認められることが多くある。これら未知ピークの同定確認に、パルプ工場排水中の有機物の一覧表は大いに役立つはずである。実際に著者らは同定確認にそれを活用している。

そこで、著者等はパルプ工場排水中の有機物の一覧表を基に、水道水中の副生成物を初めとした微量有機化合物及び水道原水中の微量有機化合物の一覧表を作成したので報告する。

なお、今回の一覧表には一般的に中沸点、高沸点である香料、多環芳香族、有機金属化合物、ダイオキシン及び関連物質、有機リン酸トリエステル、フタル酸エステル、アジピン酸エステル、農薬等の化学物質、及びそれらの光分解生成物等は未記載である。

2. 微量有機化合物の一覧表

表1に主に文献1)~4)を活用し、約1000の物質名とCas番号¹¹⁻¹³⁾及び物理化学性状¹¹⁻¹⁸⁾を記載した微量有機化合物の一覧表を示した。しかし、Cas番号が未決定、また物理化学性状が不明である物質が多くあった。文献1)は文献数61を参考にして書かれた委員会資料であり、

表 1. 微量有機化合物の一覧表

No. 1

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
脂肪族脂肪酸							
** Methanoic acid(Formic acid)	HC(=O)OH	46.03	64-18-6	8.3~8.6	100.8	1.2187	
** Methyl formate	HC(=O)OCH ₃	60.05	107-31-1		99.8		23%
** Ethanoic acid(Acetic acid)	CH ₃ COOH	60.05	64-19-7	16.6	118.1	1.049(20/4)	
*** Chloroacetic acid	CH ₂ ClCOOH	94.50	79-11-8	50~63	185~189.35	1.580(20/20)	易溶
** Dichloroacetic acid	CHCl ₂ COOH	128.94	79-43-6	9.7~13.5	192~194.4	1.563(20/4)	8.63%
** Trichloroacetic acid	CCl ₃ COOH	163.39	76-03-9	58	197.5	1.629	1.3%
Bromoacetic acid	CH ₂ BrCOOH	138.95	79-08-3	49~50	203~208	1.934(50/4)	易溶
Dibromoacetic acid	CHBr ₂ COOH	217.86	631-64-1	48	232~234		易溶
Trihaloacetic acid	CHBr ₃ COOH	296.74	75-96-7	130~133	245		
Bromochloroacetic acid	CHBrClCOOH	173.4	5589-96-8	25~38	210~212(767mmHg)	1.98480(30.6/)	
Dibromochloroacetic acid	CHBr ₂ ClCOOH	252.29	5278-95-5	89~96	232~234		
Dichlorobromoacetic acid	CHCl ₂ BrCOOH	207.84	71133-14-7	60~61	215		
+ Nitritotriacetic acid	N(CH ₂ COOH) ₃	191.14	139-13-9	230~241.5			
# Propanoic acid(Propionic acid)	CH ₃ CH ₂ COOH	74.08	79-09-4	-20.7~22.0	140~141.1	0.996(20/4)	無限
α-Chloropropionic acid(2-)	CH ₃ CHClCOOH	108.52	598-78-7	液体	186	1.265(20/4)	無限
β-Chloropropionic acid(3-)	CH ₂ ClCH ₂ COOH	108.52	107-94-8	37~42	200(765mmHg)		可溶, 易溶
α-Bromopropionic acid	CH ₃ CHBrCOOH	153.0	598-72-1	25.7	203.5	1.70(20/4)	
β-Bromopropionic acid	CH ₂ BrCH ₂ COOH	153.0	590-92-1	62.5			溶解
+ 2,2-Dichloropropionic acid	CH ₃ CCl ₂ COOH	142.97	75-99-0	98~99		1.4014(20/)	45%(25°C)
2,3-Dichloropropionic acid	ClCH ₂ CH(Cl)COOH	142.97	565-64-0	48~52	210		
2,3-Dibromopropionic acid	BrCH ₂ CH(Br)COOH	231.87	600-05-5	51~67	220~240		
Propenoic acid (Acrylic acid)	CH ₂ =CHCOOH	72.06	79-10-7	12.3~13	141~142	1.05(20/4)	無限
# Chloropropenoic acid	HC=CCOOH(:Cl, H)	106.51					
2-Chloropropenoic acid	C ₃ H ₅ ClO ₂	106.51	598-79-8	56~65	178~181	1.2115(20/)	
3-Chloropropenoic acid	C ₃ H ₅ ClO ₂	106.51	625-40-1	84~86	94(18mmHg)		
** Dichloropropenoic acid	CHCl=CClCOOH	140.96					
2,3-Dichloropropenoic acid	C ₃ H ₂ Cl ₂ O ₂	140.96	13167-36-7	78~88	103~104(2mmHg)		
3,3-Dichloropropenoic acid	C ₃ H ₂ Cl ₂ O ₂	140.96	74042-16-3				
** Trichloropropenoic acid	Cl ₂ C=CClCOOH	175.41					
- 2-Methylpropenoic acid(Methacrylic acid)	H ₂ C=C(CH ₃)COOH	86.09	79-41-4	15~16	161~163		18%
Butanoic acid(Butyric acid)	CH ₃ (CH ₂) ₃ COOH	88.11	107-92-6	-5.7~-7.9	163.5~164.5	0.960(20/4)	無限
Crotonic acid(Butenoic acid)	CH ₃ CH=CHCOOH	86.09	3724-65-0	trans 7.2 cis 15.5	199 171	0.973(72/4)	9.4%(25°C)
** Trichlorobutenoic acid	CCl ₃ CCOOH(:Cl ₃ , H ₂)	189.44					
** Tetrachlorobutenoic acid	CCl ₃ CCOOH(:Cl ₄ , H)	223.89					
Pentanoic acid(Valeric acid)	CH ₃ (CH ₂) ₄ COOH	102.13					
Trichloro-2-oxo-3-pentenoic acid	Cl ₃ CHC=CCOOH(:Cl, H)	217.44	109-52-4	-34.5	187.0	0.939(20/4)	3.7%
** 5,5,5-Trichloro-2-oxo-3-pentenoic acid	Cl ₃ CCH=CCOOH	217.44					
** 3,4,5-Tetrachloro-2-oxo-3-pentenoic acid	Cl ₃ CHCl=CClCOOH	251.88					
** Tetracloro-2-oxo-3-pentenoic acid	Cl ₃ CC=CCOOH(:Cl, H)	251.88					
** 3,4,5,5,5-Pentachloro-2-oxo-3-pentenoic acid	Cl ₃ CCCl=CClCOOH	286.33					
Caproic acid(Hexanoic acid)	CH ₃ (CH ₂) ₅ COOH	116.16	142-62-1	-3.9~-1.5	205.0	0.925(20/4)	0.89%(15°C)
Enanthic acid(Heptanoic acid)	CH ₃ (CH ₂) ₆ COOH	130.19	111-14-8	-11~-12.0	221.5~222	0.919(20/4)	0.24%
Caprylic acid(Octanoic acid)	CH ₃ (CH ₂) ₇ COOH	144.21	124-07-2	16~16.7	237.5	0.910(20/4)	不溶
Pelargonic acid(Nonanoic acid)	CH ₃ (CH ₂) ₈ COOH	158.24	112-05-0	12.5~15	254.0	0.907(20/4)	

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No. 2

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
Capric acid (decanoic acid)	$\text{CH}_3(\text{CH}_2)_8\text{COOH}$	172.27	334-48-5	31~31.5	268.4~269.0	0.893(32/4)	
Undecylic acid (undecanoic acid)	$\text{CH}_3(\text{CH}_2)_9\text{COOH}$	186.30	112-37-8	29.3	284.0	0.827(20/4)	
Lauric acid (dodecanoic acid)	$\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$	200.32	143-07-7	44~44.2	298.9	1.0099(35/4)	
Tridecyl acid (tridecanoic acid)	$\text{CH}_3(\text{CH}_2)_{11}\text{COOH}$	214.35	638-53-9	41			
Myristic acid (tetradecanoic acid)	$\text{CH}_3(\text{CH}_2)_{12}\text{COOH}$	228.38	544-63-8	53.5~53.9	326.2	0.8584(60/)	
Pentadecylic acid (pentadecanoic acid)	$\text{CH}_3(\text{CH}_2)_{13}\text{COOH}$	242.40	1002-84-2	53			
Palmitic acid (hexadecanoic acid)	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$	256.43	57-10-3	60~63.1	351.5		
Margaric acid (heptadecanoic acid)	$\text{CH}_3(\text{CH}_2)_{15}\text{COOH}$	270.46	506-12-7	61.1	227(100mmHg)		
Stearic acid (octadecanoic acid)	$\text{CH}_3(\text{CH}_2)_{16}\text{COOH}$	284.49	57-11-4	69.6~71	376.1	0.848(70/)	0.03%(25°C)
Nonadecylic acid (nonadecanoic acid)	$\text{CH}_3(\text{CH}_2)_{17}\text{COOH}$	298.51	646-30-0	68			
Arachidic acid (eicosanoic acid)	$\text{CH}_3(\text{CH}_2)_{18}\text{COOH}$	312.54	506-30-9	76.1~76.3	328(分解)		
Heneicosanoic acid	$\text{CH}_3(\text{CH}_2)_{19}\text{COOH}$	326.56	2363-71-5	75			
Behenic acid (docosanoic acid)	$\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$	340.59	112-85-6	80.02	306(60mmHg)		
Oleic acid	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$	282.47	112-80-1	14	233(15mmHg)		不溶
10-Hydroxystearic acid	$\text{CH}_3(\text{CH}_2)_7\text{CH}(\text{OH})(\text{CH}_2)_6\text{COOH}$	300.48	638-26-6	82			
12-Hydroxystearic acid	$\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{OH})(\text{CH}_2)_8\text{COOH}$	300.48	106-14-9	78			
Dihydroxystearic acid	$\text{C}_{17}\text{H}_{32}\text{O}_4$	316.5	26248-43-1				
erythro-6,7-Dihydroxystearic acid	$\text{C}_{17}\text{H}_{32}\text{O}_4$	316.5	14073-16-6				
threo-6,7-Dihydroxystearic acid	$\text{C}_{17}\text{H}_{32}\text{O}_4$	316.5	13985-16-5				
8,9-Dihydroxystearic acid	$\text{CH}_3(\text{CH}_2)_6[\text{CH}(\text{OH})]_2(\text{CH}_2)_6\text{COOH}$	316.5	120-87-6				
9,10-Dihydroxystearic acid	$\text{CH}_3(\text{CH}_2)_7[\text{CH}(\text{OH})]_2(\text{CH}_2)_7\text{COOH}$	316.5	31328-13-9				
10,18-Dihydroxystearic acid	$\text{C}_{17}\text{H}_{32}\text{O}_4$	316.5	2443-39-2	cis59.5~59.8 trans55.3			
9,10-Epoxyoctadecanoic acid	$[\text{CH}(\text{CH}_2)_7\text{COOH}]_2\text{O}$	298.5					
threo-9,10(10,9)-Chloro-hydroxystearic acid	$\text{CH}_3[(\text{CH}_2)_7\text{CH}(\text{Cl})\text{OH}]_2\text{COOH}$	359.35					
Dichlorostearic acid	$\text{C}_{17}\text{H}_{31}\text{Cl}_2\text{O}_2$	353.38	31135-63-4				
2,2-Dichlorostearic acid	$\text{C}_{17}\text{H}_{31}\text{Cl}_2\text{O}_2$	353.38	56279-50-6				
9,10-Dichlorostearic acid	$\text{C}_{17}\text{H}_{31}\text{Cl}_2\text{O}_2$	353.38	5829-48-1				
Glycolic acid	$\text{CH}_2(\text{OH})\text{COOH}$	76.05	79-14-1	79	分解		無限
Lactic acid	$\text{C}_3\text{H}_6\text{O}_3$	90.08	50-21-5				
D-Lactic acid	$\text{CH}_3\text{CH}(\text{OH})\text{COOH}$	90.08	10326-41-7	52.8	分解		無限
L-Lactic acid	$\text{CH}_3\text{CH}(\text{OH})\text{COOH}$	90.08	79-33-4				
DL-Lactic acid	$\text{CH}_3\text{CH}(\text{OH})\text{COOH}$	90.08	598-82-3	18	119(12mmHg)	1.240	無限
2-Hydroxypropanoic acid	$\text{C}_3\text{H}_6\text{O}_3$	90.08	50-21-5				
3-Hydroxypropanoic acid	$\text{CH}_2(\text{OH})\text{CH}_2\text{COOH}$	90.08	503-66-2				
Glyceric acid	$\text{CH}_2(\text{OH})\text{CH}(\text{OH})\text{COOH}$	106.08	473-81-4	液体	分解		無限
DL-Glyceric acid	$\text{HOCH}_2\text{CH}(\text{OH})\text{COOH}$	106.08	600-19-1				
2,3-Dihydroxybutanoic acid	$\text{C}_4\text{H}_8\text{O}_4$	120.11	3413-97-6				
2,4-Dihydroxybutanoic acid	$\text{C}_4\text{H}_8\text{O}_4$	120.11	1518-62-3				
(S)-3,4-Dihydroxybutanoic acid	$\text{C}_4\text{H}_8\text{O}_4$	120.11	51267-44-8				
3-4-Dihydroxybutanoic acid	$\text{CH}_3(\text{OH})\text{CH}(\text{OH})\text{CH}_2\text{COOH}$	120.11	1518-61-2				
Threonic acid	$\text{CH}_2(\text{OH})[\text{CH}(\text{OH})]_2\text{COOH}$	136.11	3909-12-4				
Erythronic acid	$\text{CH}_2(\text{OH})[\text{CH}(\text{OH})]_2\text{COOH}$	136.11	13752-84-6				
3-Deoxythreopentonic acid	$\text{CH}_2(\text{OH})\text{CH}(\text{OH})\text{CH}_2\text{CH}(\text{OH})\text{COOH}$	150.14	1518-60-1				
3-Deoxyerythrophentonic acid	$\text{CH}_2(\text{OH})\text{CH}(\text{OH})\text{CH}_2\text{CH}(\text{OH})\text{COOH}$	150.14					
Arabinonic acid	$\text{CH}_2(\text{OH})[\text{CH}(\text{OH})]_3\text{COOH}$	166	13752-83-5				

表 1. 微量有機化合物の一覧表

No.3

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
D-Arabinonic acid	C ₅ H ₁₀ O ₆	166	488-30-2				
L-Arabinonic acid	C ₅ H ₁₀ O ₆	166	608-53-7	118~119			
Glucosaccharinic acid	C ₆ H ₁₂ O ₆	180.16	66702-03-2				
α-Glucosaccharinic acid	CH ₂ (OH)CH(OH)(OH)CH ₂ C(OH)(OH)COOH	180.16	1518-54-3				
β-Glucosaccharinic acid	CH ₂ (OH)CH(OH)CH ₂ C(OH)(OH)COOH	180.16	1518-56-5				
Oxalic acid	(COOH) ₂	90.04	144-62-7	101.5	昇華	1.653(19/4)	
Malonic acid	HOOCCH ₂ COOH	104.07	141-82-2	133~135		1.631(15/4)	150%
Chloromalonic acid	HOOCCHClCOOH	138.51	600-336-9				
Succinic acid	HOOCCH ₂ CH ₂ COOH	118.09	110-15-6	183~185	251~235	1.564(15/4)	6.8%
Chlorosuccinic acid	HOOCCH ₂ CHClCOOH	152.53					
Dichlorosuccinic acid	HOOCCHCl ₂ CH ₂ COOH	186.97					
Methylsuccinic acid	HOOCCH ₂ CH(CH ₃)COOH	132.12	498-21-5	111	200	1.411	
Tartaric acid	C ₄ H ₆ O ₆	150.09	87-68-4	169~170		1.7598	溶解
D-Tartaric acid	HOOCCH(OH)CH(OH)COOH	150.09	147-71-7	168~170	分解	1.759(20/4)	135%(20°C)
L-Tartaric acid	HOOCCH(OH)CH(OH)COOH	150.09	87-69-4	168~170	分解	1.759(20/4)	135%(20°C)
DL-Tartaric acid	HOOCCH(OH)CH(OH)COOH·H ₂ O	168.11	133-37-9	205~206		1.697(20/4)	
Hydroxysuccinic acid(Malic acid)	C ₄ H ₆ O ₅	134.09	6915-15-7				
D-Malic acid	HOOCCH(OH)CH ₂ COOH	134.09	636-61-3	98~102			
DL-Malic acid	HOOCCH(OH)CH ₂ COOH	134.09	617-48-1	131~133	150(分解)	1.601(20/4)	55.8%(20°C)
L-Malic acid	HOOCCH(OH)CH ₂ COOH	134.09	97-67-6	100~103	140(分解)	1.595(20/4)	36.35%(20°C)
Fumaric acid	HOOCCH=CHCOOH	116.07	110-17-8	286~290	昇華	1.625	0.63%
Chlorofumaric acid	HOOCCH=CClCOOH	150.53	617-42-5	193	昇華		易溶
Dichlorofumaric acid	HOOCCH=CCl ₂ COOH	184.97					
Maleic acid	HOOCCH=CHCOOH	116.08	110-16-7	130	135	1.590	78.8%
Chloromaleic acid	HOOCCH=CClCOOH	150.53	617-43-6	108	180(無水)		
Dichloromaleic acid	C ₄ H ₂ Cl ₂ O ₄	184.97	608-42-4	112~120			
α,β-Dichloromaleic acid	HOOCCH=CCl ₂ COOH	184.97	608-42-4				
2,3-Dichloromaleic acid	HOOCCH=CCl ₂ COOH	184.97	608-42-4				
芳香族脂肪酸							
Benzoic acid	C ₆ H ₅ COOH	122.12	65-85-0	121~124	249.2	1.2659	0.21%(25°C)
o-Chlorobenzoic acid	ClC ₆ H ₄ COOH	156.57	118-91-2	140~143	昇華	1.544(20/4)	0.23%
m-Chlorobenzoic acid	ClC ₆ H ₄ COOH	156.57	535-80-8	151~156	昇華	1.496(25/)	0.5%
p-Chlorobenzoic acid	ClC ₆ H ₄ COOH	156.57	74-11-3	239~243	昇華		
2-Bromobenzoic acid (o-)	BrC ₆ H ₄ COOH	201.02	88-65-3	146~151	昇華	1.929(20/)	微溶
3-Bromobenzoic acid (m-)	BrC ₆ H ₄ COOH	201.02	585-76-2	155	> 280	1.845(20/)	微溶
4-Bromobenzoic acid (p-)	BrC ₆ H ₄ COOH	201.02	586-76-5	254		1.894(20/)	難溶
2,3-Dichlorobenzoic acid	Cl ₂ C ₆ H ₃ COOH	191.01	50-45-3	168.2			
2,4-Dichlorobenzoic acid	Cl ₂ C ₆ H ₃ COOH	191.01	50-84-0	161~165	昇華		不溶
2,5-Dichlorobenzoic acid	Cl ₂ C ₆ H ₃ COOH	191.01	50-79-3	154~157	301		0.083%
2,6-Dichlorobenzoic acid	Cl ₂ C ₆ H ₃ COOH	191.01	50-30-6	143.7	昇華		
3,4-Dichlorobenzoic acid	Cl ₂ C ₆ H ₃ COOH	191.01	51-44-5	205~209			
3,5-Dichlorobenzoic acid	Cl ₂ C ₆ H ₃ COOH	191.01	51-36-5	188	昇華		難溶
4-Bromo-2-chlorobenzoic acid	BrClC ₆ H ₃ COOH	235.46	59748-90-2				
5-Bromo-2-chlorobenzoic acid	BrClC ₆ H ₃ COOH	235.46	21739-92-4	158			

表 1. 微量有機化合物の一覧表

No. 4

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
Salicylic acid	$\text{HO}_2\text{C}_6\text{H}_4\text{COOH}$	138.13	69-72-7	158~161	76(昇華)	1.443(20/)	0.16%
m-Hydroxybenzoic acid	$\text{HO}_2\text{C}_6\text{H}_4\text{COOH}$	138.13	99-06-9	201~205		1.473	0.84%
p-Hydroxybenzoic acid	$\text{HO}_2\text{C}_6\text{H}_4\text{COOH}$	138.13	99-96-7	213~217	分解	1.497(20/)	0.4%
3,5-Dichloro-2-hydroxybenzoic acid	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})\text{COOH}$	207.01	320-72-9				
3,5-Dichloro-4-hydroxybenzoic acid	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})\text{COOH}$	207.01	3336-41-2				
Chloro-3,4-dihydroxybenzoic acid	$\text{ClC}_6\text{H}_2(\text{OH})_2\text{COOH}$	188.57					
Dichloro-3,4-dihydroxybenzoic acid	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2\text{COOH}$	223.01					
Trichloro-3,4-dihydroxybenzoic acid	$\text{Cl}_3(\text{OH})_2\text{C}_6\text{COOH}$	257.56					
o-Nitrobenzoic acid	$\text{NO}_2\text{C}_6\text{H}_4\text{COOH}$	167.12	552-16-9	144~149		1.575	0.65%
m-Nitrobenzoic acid	$\text{NO}_2\text{C}_6\text{H}_4\text{COOH}$	167.12	121-92-6	140~144		1.494	0.3%
p-Nitrobenzoic acid	$\text{NO}_2\text{C}_6\text{H}_4\text{COOH}$	167.12	62-23-7	240以上	昇華	1.610(20/4)	0.03%
3-Nitrophthalic acid	$\text{NO}_2\text{C}_6\text{H}_3(\text{COOH})_2$	211.13	603-11-2	222			可溶
4-Nitrophthalic acid	$\text{NO}_2\text{C}_6\text{H}_3(\text{COOH})_2$	211.13	610-27-5	165			易溶
Nitroterephthalic acid	$\text{NO}_2\text{C}_6\text{H}_3(\text{COOH})_2$	211.13	610-29-7	270			
2,3-Dimethylbenzoic acid	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{COOH}$	150.2	603-79-2	144.5~144.8			
2,4-Dimethylbenzoic acid	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{COOH}$	150.2	611-01-8	125.4~125.8	267(72mmHg)		
2,5-Dimethylbenzoic acid	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{COOH}$	150.2	610-72-0	133.8~134.1	268		
2,6-Dimethylbenzoic acid	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{COOH}$	150.2	632-46-2	115.8~116.2	155~160(17mmHg)		
3,4-Dimethylbenzoic acid	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{COOH}$	150.2	619-04-5	167.4~168.2	昇華		
3,5-Dimethylbenzoic acid	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{COOH}$	150.2	499-06-9	171.6~172	昇華		
p-Butylbenzoic acid	$\text{C}_4\text{H}_9\text{C}_6\text{H}_4\text{COOH}$	178.23	20651-71-2				
p-tert-Butylbenzoic acid	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{COOH}$	178.23	98-73-7	163~167			微溶
Vanillic acid	$\text{CH}_3\text{O}(\text{OH})\text{C}_6\text{H}_3\text{COOH}$	168.15	121-34-6	211~212	昇華		0.12%
o-Vanillic acid	$\text{CH}_3\text{O}(\text{OH})\text{C}_6\text{H}_3\text{COOH}$	168.15	877-22-5				
Chlorovanillic acid	$\text{ClCH}_3\text{O}(\text{OH})\text{C}_6\text{H}_2\text{COOH}$	202.59					
5-Chlorovanillic acid	$\text{C}_6\text{H}_4\text{ClO}_4$	202.59	62936-23-6				
Dichlorovanillic acid	$\text{Cl}_2\text{CH}_3\text{O}(\text{OH})\text{C}_6\text{HCOOH}$	237.04					
Trichlorovanillic acid	$\text{Cl}_3\text{CH}_3\text{O}(\text{OH})\text{C}_6\text{COOH}$	271.48					
Ferulic acid	$\text{HO}_2\text{C}_6\text{H}_3(\text{OCH}_3)\text{CH}:\text{CHCOOH}$	194.19	1135-24-6	169~175	分解		不溶
5-Chloroferulic acid	$\text{ClCH}_3\text{O}(\text{OH})\text{C}_6\text{H}_2\text{CH}:\text{CHCOOH}$	228.64	5438-40-4				
Syringic acid	$(\text{CH}_3\text{O})_2(\text{OH})\text{C}_6\text{H}_2\text{COOH}$	198.18	530-57-4				
Dichlorosyringic acid	$\text{Cl}_2(\text{CH}_3\text{O})_2(\text{OH})\text{C}_6\text{COOH}$	267.06	20624-96-8				
Dichloro-3,5-dimethoxy-4-hydroxyphenylglyoxylic acid	$\text{Cl}_2(\text{CH}_3\text{O})_2(\text{OH})\text{C}_6\text{CH}_2\text{COOH}$	281.09					
Dichloro-3,5-dimethoxy-4-hydroxymandelic acid	$\text{Cl}_2(\text{CH}_3\text{O})_2(\text{OH})\text{C}_6\text{COOH}$	295.07					
2-Furancarboxylic acid	$\text{Cl}_2(\text{CH}_3\text{O})_2(\text{OH})\text{C}_6\text{CH}(\text{OH})\text{COOH}$	297.09					
3-Furancarboxylic acid	$\text{C}_4\text{H}_3\text{O}(\text{COOH})$	112.08	88-14-2	132			
2-Thiophenecarboxylic acid	$\text{C}_4\text{H}_3\text{O}(\text{COOH})$	112.08	488-93-7	122			
3-Thiophenecarboxylic acid	$\text{C}_4\text{H}_3\text{S}(\text{COOH})$	128.15	527-72-0	128.5			
4-Thiophenecarboxylic acid	$\text{C}_4\text{H}_3\text{S}(\text{COOH})$	128.15	88-13-1	138			
Dichloro-2-Thiophene-carboxylic acid	$\text{Cl}_2\text{C}_4\text{H}_2\text{S}(\text{COOH})$	162.58					
Abietic acid	$\text{Cl}_2\text{C}_4\text{HS}(\text{COOH})$	197.03					
Dehydroabietic acid	$\text{C}_{20}\text{H}_{30}\text{O}_2$	302.46	514-10-3	172~175			不溶
(-)-Dehydroabietic acid	$\text{C}_{20}\text{H}_{28}\text{O}_2$	301.43	1740-19-8				
(+)-Dehydroabietic acid	$\text{C}_{20}\text{H}_{28}\text{O}_2$	301.43	1740-19-8				
		301.43	35949-24-7				

表 1. 微量有機化合物の 一覧表

No. 5

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
* 6,8,11,13-Dehydrodihydroabietic acid	C ₂₀ H ₂₄ O ₂	296.39					
3-Oxodehydroabietic acid	C ₂₀ H ₂₄ O ₃	314.43	23655-33-6				
# 7-Oxodehydroabietic acid	C ₂₀ H ₂₄ O ₃	314.43	18684-55-4				
** Chlorodehydroabietic acid	C ₂₀ H ₂₄ O ₃	335.88	57055-38-6				
* 12-Chlorodehydroabietic acid	C ₂₀ H ₂₂ O ₂ Cl	335.88	65310-45-4				
* 14-Chlorodehydroabietic acid	C ₂₀ H ₂₂ O ₂ Cl	335.88	58948-12-2				
** Dichlorodehydroabietic acid	C ₂₀ H ₂₀ O ₂ Cl ₂	370.32	57055-39-7				
* 12,14-Dichlorodehydroabietic acid	C ₂₀ H ₂₀ O ₂ Cl ₂	370.32	65281-77-8				
** Isopimaric acid	C ₂₀ H ₃₀ O ₂	302.44	5835-26-7	16			
** Pimaric acid	C ₂₀ H ₃₀ O ₂	302.44	127-27-5	217~219	282(18mmHg)		
** Palustic acid	C ₂₀ H ₃₀ O ₂	302.44	1945-53-5	162~167			
*- o-Benzenedicarboxylic acid	C ₆ H ₄ (COOH) ₂	166.13	88-99-3	191~203(234)	分解	1.59	
*- m-Benzenedicarboxylic acid	C ₆ H ₄ (COOH) ₂	166.13	121-91-5	345~352			不溶
** p-Benzenedicarboxylic acid	C ₆ H ₄ (COOH) ₂	166.13	100-21-0		300(昇華)		不溶
** Chlorothiophenedicarboxylic acid	ClC ₆ HS(COOH) ₂	206.6					
# Phthalic anhydride	C ₈ H ₄ (CO) ₂ O	150.14	85-44-9	130.8~131.8	285	1.527	不溶
o-Phthalic anhydride	C ₈ H ₄ (CO) ₂ O	150.14		100.5		1.404	易溶
m-Phthalic anhydride	C ₈ H ₄ (CO) ₂ O	150.14		175			可溶
p-Phthalic anhydride	C ₈ H ₄ (CO) ₂ O	150.14		256	昇華		
Dichloromaleic anhydride	C ₆ Cl ₂ O ₃	166.96	1122-17-4	117~123	184~186(745mmHg)		
2,3-Dichloromaleic anhydride	C ₆ Cl ₂ O ₃	166.96					
3,4-Dichloromaleic anhydride	C ₆ Cl ₂ O ₃	166.96	1122-17-4				
2-Chloro-3-methylmaleic anhydride	C ₈ H ₆ ClO ₃	146.54					
Chloromethylmaleic anhydride	C ₈ H ₆ ClO ₃	146.54	41702-49-2				
1-Naphthylacetic acid	C ₁₁ H ₇ CH ₂ COOH	186.21	86-87-3	131~135.5			0.036%
2-Naphthylacetic acid	C ₁₁ H ₇ CH ₂ COOH	186.21	581-96-4	140~144			
* Antiseptodecanoic acid	C ₁₇ H ₃₄ O ₂	270.44	5918-29-6				
* Linoleic acid	C ₁₈ H ₃₂ O ₂	280.45	60-33-3	-14~-5	229~300(16mmHg)	0.9025(20/4)	不溶
* Linolenic acid	C ₁₈ H ₃₀ O ₂	278.42	463-40-1		197(4mmHg)	0.905(20/4)	
* Lipoic acid	C ₈ H ₁₄ O ₂	388.62					
* Piolenic acid	C ₁₈ H ₃₀ O ₂	278.42					
* Chloromethoxyprotocatechuic acid	C ₈ H ₇ O ₅ Cl	218.59					
フェノール							
Phenol	C ₆ H ₅ OH	94.11	108-95-2	40.8~40.9	181.75~182.2	1.071(20/4)	可溶
*- o-Chlorophenol	ClC ₆ H ₄ OH	128.56	95-57-8	8.7~8.8	175.6	1.235(25/4)	2.8%
*- m-Chlorophenol	ClC ₆ H ₄ OH	128.56	108-43-0	32.8	214	1.268(25/4)	2.6%
*- o-Bromophenol	BrC ₆ H ₄ OH	173.02	95-56-7	5.6	194~195	1.553(80/4)	不溶
*- m-Bromophenol	BrC ₆ H ₄ OH	173.01	591-20-8	32~33	236~237	1.610(20/4)	不溶
*- p-Bromophenol	BrC ₆ H ₄ OH	173.01	106-41-2	63~67	235~236	1.558(80/4)	1.4%
* Chlorocymene- α -o ^s	ClCH ₂ CH(CH ₃) ₂ C ₆ H ₄ OH	184.67					
* Bromocymene- α -o ^s	BrCH ₂ CH(CH ₃) ₂ C ₆ H ₄ OH	229.13	92067-00-0				
* 2,3-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	576-24-9	54~60		1.38	0.45%
*- 2,4-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	120-83-2	43~45			難溶
*- 2,5-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	583-78-8	54~58	209~211		
*- 2,6-Dichlorophenol	Cl ₂ C ₆ H ₃ OH	163.00	87-65-0	63~68	211(744mmHg)		
					218~220		

表 1. 微量有機化合物の一覧表

化合物名 (英語名)	化学式	分子量	Cas 番号	融点	沸点	比重	水への溶解性
*- 3,4-Dichlorophenol	$\text{Cl}_2\text{C}_6\text{H}_3\text{OH}$	163.00	95-77-2	65~69	253.5(767mmHg)		難溶
*- 3,5-Dichlorophenol	$\text{Cl}_2\text{C}_6\text{H}_3\text{OH}$	163.00	591-35-5	65~69	233		難溶
* 2,3,6-Trichlorophenol	$\text{Cl}_3\text{C}_6\text{H}_2\text{OH}$	197.45	933-75-5	58	253		微溶
** 2,4,5-Trichlorophenol	$\text{Cl}_3\text{C}_6\text{H}_2\text{OH}$	197.45	95-95-4	63~69			
** 2,4,6-Trichlorophenol	$\text{Cl}_3\text{C}_6\text{H}_2\text{OH}$	197.45	88-06-2	65~69.5	246	1.4901(75/4)	0.09%
- 2,4,6-Tribromophenol	$\text{Br}_3\text{C}_6\text{H}_2\text{OH}$	330.80	118-79-6	92.94~96	244		0.00433%
* 2,3,4,5-Tetrachlorophenol	$\text{Cl}_4\text{C}_6\text{H}_2\text{OH}$	231.9	4901-51-3	> 300			
** 2,3,4,6-Tetrachlorophenol	$\text{Cl}_4\text{C}_6\text{H}_2\text{OH}$	231.9	58-90-2				
* 2,3,5,6-Tetrachlorophenol	$\text{Cl}_4\text{C}_6\text{H}_2\text{OH}$	231.9	935-95-5				
** Pentachlorophenol	$\text{C}_6\text{Cl}_5\text{OH}$	266.34	87-86-5	189~191	309~310		
- o-Methyl phenol	$\text{CH}_3\text{C}_6\text{H}_4\text{OH}$	108.14	95-48-7	30.94~32	190.95~191.1	1.0465(20/4)	2.6%
- m-Methyl phenol	$\text{CH}_3\text{C}_6\text{H}_4\text{OH}$	108.14	108-39-4	10.9~11.5	202.2	1.0336(20/4)	0.53%
- p-Methyl phenol	$\text{CH}_3\text{C}_6\text{H}_4\text{OH}$	108.14	106-44-5	34.78~36.5	201.88~202.5	1.0341(20/4)	1.8%
- 4-Chloro-2-methylphenol	$\text{ClC}_6\text{H}_3(\text{CH}_3)\text{OH}$	142.58	1570-64-5	45~50	220~225		
- 4-Chloro-3-methylphenol	$\text{ClC}_6\text{H}_3(\text{CH}_3)\text{OH}$	142.58	59-50-7	64~68	235		
- 6-Chloro-3-methylphenol	$\text{ClC}_6\text{H}_3(\text{CH}_3)\text{OH}$	142.58	615-74-7	45~49	196		
- 6-tert-Butyl-o-cresol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)\text{OH}$	164.25	2219-82-1	32	230	0.995 (40/)	
- 6-tert-Butyl-m-cresol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)\text{OH}$	164.25	88-60-8				
- 2-tert-Butyl-p-cresol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)\text{OH}$	164.25	2409-55-4				
- o-Ethyl phenol	$\text{C}_2\text{H}_5\text{C}_6\text{H}_4\text{OH}$	122.17	90-00-6	< -18	207(756mmHg)	1.021 (20/4)	難溶
- m-Ethyl phenol	$\text{C}_2\text{H}_5\text{C}_6\text{H}_4\text{OH}$	122.17	620-17-7	-4.6	214	1.02	微溶
- p(4)-Ethyl phenol	$\text{C}_2\text{H}_5\text{C}_6\text{H}_4\text{OH}$	122.17	123-07-9	43~46	219	1.0123(20/)	微溶
- 2-Propyl phenol(o-)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_3\text{OH}$	136.19	644-35-9	7	221.5~220.0	1.00~1.02(20/)	
- 3-Isopropyl phenol	$(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{OH}$	136.19	618-45-1	21~31	228.0		
- 4-Isopropyl phenol	$(\text{CH}_3)_2\text{CHC}_6\text{H}_4\text{OH}$	136.19	99-89-8	58~84	228~230(745mmHg)	0.96~0.99(20/)	
- 2,3-Dimethyl phenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	526-75-0	71~75	218		
- 2,4-Dimethyl phenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	105-67-9	25.4~28	210	1.028 (14/4)	難溶
- 2,5-Dimethyl phenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	95-87-4	73~77	212	1.169	溶解
- 2,6-Dimethyl phenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	576-26-1	45~49	203		熱湯に可溶
- 3,4-Dimethyl phenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	95-65-8	62.5~67	225(757mmHg)	1.023	微溶
- 3,5-Dimethyl phenol	$(\text{CH}_3)_2\text{C}_6\text{H}_3\text{OH}$	122.17	108-68-9	62~65	220		
- 2,3,5-trimethyl phenol	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{OH}$	136.19	2416-94-6	60~63			
- 2,4,5-trimethyl phenol	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{OH}$	136.19	496-78-6	72	232		
- 2,4,6-trimethyl phenol	$(\text{CH}_3)_3\text{C}_6\text{H}_2\text{OH}$	136.19	527-60-6	70.4~71.6	221		
- 4-Nonylphenol	$\text{C}_9\text{H}_{19}\text{C}_6\text{H}_4\text{OH}$	220.35	104-40-5			0.95	
- Catechol	$\text{C}_6\text{H}_4(\text{OH})_2$	110.11	120-80-9	105	240~245	1.344(20/4)	45%
- Hydroquinone	$\text{C}_6\text{H}_4(\text{OH})_2$	110.11	123-31-9	170.3~174	285(730mmHg)	1.330	易溶
- Resorcinol	$\text{C}_6\text{H}_4(\text{OH})_2$	110.11	108-46-3	110~112	280.8~281	1.285(15/4)	280%(20°C)
- 3-Chlorocatechol	$\text{ClC}_6\text{H}_3(\text{OH})_2$	144.56	4018-65-9	45~71	136~138(20mmHg)		
- 4-Chlorocatechol	$\text{ClC}_6\text{H}_3(\text{OH})_2$	144.56	2138-22-9	88			
- 4-Chlororesorcinol	$\text{ClC}_6\text{H}_3(\text{OH})_2$	144.56	95-88-5	107			
- Dichlorocatechol	$\text{C}_6\text{H}_2\text{Cl}_2\text{O}_2$	179	25167-85-5				
* 3,4-Bichlorocatechol	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2$	179	3978-67-4	99.00			
* 3,5-Bichlorocatechol	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2$	179	13673-92-2	83~87.5			
- 3,6-Dichlorocatechol	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2$	179	3938-16-7	109.0~111.0			
- 4,5-Dichlorocatechol	$\text{Cl}_2\text{C}_6\text{H}_2(\text{OH})_2$	179	3428-24-8	105~117			

表 1. 微量有機化合物の一覧表

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
** Trichlorocatechol	C ₆ H ₃ Cl ₃ O ₂	213.46	25167-84-4				
* 3,4,5-Trichlorocatechol	Cl ₃ C ₆ H(OH) ₂	213.46	56961-20-7				
* 3,4,6-Trichlorocatechol	Cl ₃ C ₆ H(OH) ₂	213.46	32139-72-3				
** Tetrachlorocatechol	C ₆ H ₂ Cl ₄ O ₂	247.89	1198-55-6				
* 3,3,5,6-Tetrachlorocatechol	Cl ₄ C ₆ (OH) ₂	247.89	1198-55-6				
# Chloroethylcatechol	Cl(CH ₂ CH ₂)C ₆ H ₂ (OH) ₂	172.62					
# Dichloroethylcatechol	Cl ₂ (CH ₂ CH ₂)C ₆ H(OH) ₂	207.07					
# Dichlorobutylcatechol	Cl ₂ (CH ₂) ₃ CH ₂ C ₆ H(OH) ₂	235.12					
2,3-Dichlorohydroquinone	Cl ₂ C ₆ H ₂ (OH) ₂	143.56	608-44-6				
2,5-Dichlorohydroquinone	Cl ₂ C ₆ H ₂ (OH) ₂	143.56	824-69-1				
2,6-Dichlorohydroquinone	Cl ₂ C ₆ H ₂ (OH) ₂	143.56	20103-10-0				
* o-Methoxyphenol (o-Guaiacol)	CH ₃ OC ₆ H ₄ OH	124.14	90-05-1	28.3	205	1.135(20/4)	1.88%
* m-Methoxyphenol	CH ₃ OC ₆ H ₄ OH	124.14	150-19-6	-17.5	245.2	1.145(20/4)	
* p-Methoxyphenol	CH ₃ OC ₆ H ₄ OH	124.14	150-76-5	55~58	243		
** Chloroguaiacol	C ₇ H ₇ ClO ₂	158.6					
3-Chloroguaiacol	Cl(CH ₃ O)C ₆ H ₃ OH	158.6	77102-92-2	31.5~33.0			
4-Chloroguaiacol	Cl(CH ₃ O)C ₆ H ₃ OH	158.6	16766-30-6	16~17	241~243		0.5%(25°C)
5-Chloroguaiacol	Cl(CH ₃ O)C ₆ H ₃ OH	158.6	3743-23-5	34~37	237~239		0.39%(25°C)
6-Chloroguaiacol	Cl(CH ₃ O)C ₆ H ₃ OH	158.6	72403-03-3	54			
** Dichloroguaiacol	C ₇ H ₆ Cl ₂ O ₂	193.04	65724-16-5				
3,4-Dichloroguaiacol	Cl ₂ (CH ₃ O)C ₆ H ₂ OH	193.04	77102-94-4	59~64			
3,5-Dichloroguaiacol	Cl ₂ (CH ₃ O)C ₆ H ₂ OH	193.04	56880-89-8	70			
3,6-Dichloroguaiacol	Cl ₂ (CH ₃ O)C ₆ H ₂ OH	193.04	77102-93-3	69~73			
4,5-Dichloroguaiacol	Cl ₂ (CH ₃ O)C ₆ H ₂ OH	193.04	2460-49-3	63~65	260~270		0.575%(25°C)
4,6-Dichloroguaiacol	Cl ₂ (CH ₃ O)C ₆ H ₂ OH	193.04	16766-31-7				0.7%(25°C)
5,6-Dichloroguaiacol	Cl ₂ (CH ₃ O)C ₆ H ₂ OH	193.04	77102-95-5				
Trichloroguaiacol	C ₇ H ₅ Cl ₃ O ₂	227.49	61966-36-7				
* 3,4,5-Trichloroguaiacol	Cl ₃ (CH ₃ O)C ₆ HOH	227.49	57057-83-7				
* 3,4,6-Trichloroguaiacol	Cl ₃ (CH ₃ O)C ₆ HOH	227.49	60712-44-9				
* 3,5,6-Trichloroguaiacol	Cl ₃ (CH ₃ O)C ₆ HOH	227.49	938-23-8				
** 4,5,6-Trichloroguaiacol	Cl ₃ (CH ₃ O)C ₆ HOH	227.49	2668-24-8				
* Tetrachloroguaiacol	Cl ₄ (CH ₃ O)C ₆ OH	261.93	2539-17-5				
* 3,4,5,6-Tetrachloroguaiacol	Cl ₄ (CH ₃ O)C ₆ OH	261.93	2539-17-5				
* 3,5-Dichloro-2,6-dimethoxyphenol	Cl ₂ (CH ₃ O) ₂ C ₆ H ₂ OH	223.06					
* 3,4,5-Trichloro-2,6-dimethoxyphenol	Cl ₃ (CH ₃ O) ₂ C ₆ OH	257.5	2539-26-6				
* Chloro-1,2,3-trihydroxybenzene	ClC ₆ H ₂ (OH) ₃	160.56					
* Chloro-1,2,4-trihydroxybenzene	ClC ₆ H ₂ (OH) ₃	160.56					
** Dichloro-1,2,3-trihydroxybenzene	Cl ₂ C ₆ H(OH) ₃	195.01					
** Dichloro-1,2,4-trihydroxybenzene	Cl ₂ C ₆ H(OH) ₃	195.01					
** Trichloro-1,2,3-trihydroxybenzene	Cl ₃ C ₆ (OH) ₃	229.45					
** Trichloro-1,2,4-trihydroxybenzene	Cl ₃ C ₆ (OH) ₃	229.45					
* Chlorodihydroxy-methoxybenzene	Cl(CH ₃ O)C ₆ H ₂ (OH) ₂	174.59					
# Dichlorodihydroxy-methoxybenzene	Cl ₂ (CH ₃ O)C ₆ H(OH) ₂	209.04	75562-93-5				
# Syringol (Dimethoxyphenol)	(CH ₃ O) ₂ C ₆ H ₃ OH	154.17					
* 2,6-Dimethoxyphenol	(CH ₃ O) ₂ C ₆ H ₃ OH	154.17	91-10-1	56			
* 3,5-Dimethoxyphenol	(CH ₃ O) ₂ C ₆ H ₃ OH	154.17	500-99-2	45			

表 1. 微量有機化合物の一覧表

No. 8

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
# Dichlorosyringol	$\text{Cl}_2(\text{CH}_3\text{O})_2\text{C}_6\text{H}_4\text{OH}$	223.07					
3,5-Dichlorosyringol	$\text{Cl}_2(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3(\text{OH})$	223.07	78782-46-4				
* Trichlorosyringol	$\text{Cl}_3(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3(\text{OH})$	257.5	2539-26-6				
# 3,4,5-Trichlorosyringol	$\text{Cl}_3(\text{CH}_3\text{O})_2\text{C}_6\text{H}_3(\text{OH})$	257.5	2539-26-6				
- o-Nitrophenol	$\text{NO}_2\text{C}_6\text{H}_4\text{OH}$	139.11	88-75-5	44.5~47.5	214~217.5	1.657(25/)	微溶, 熱湯に可溶
- m-Nitrophenol	$\text{NO}_2\text{C}_6\text{H}_4\text{OH}$	139.11	554-84-7	96~99	194(70mmHg)	1.485(20/4)	難(高)溶
+ p-Nitrophenol	$\text{NO}_2\text{C}_6\text{H}_4\text{OH}$	139.11	100-02-7	113~116	273	1.479~1.495(20/4)	0.84%(15°C)
- 2-Methyl-3-nitrophenol	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2\text{OH}$	153.14	5460-31-1	140~147	180(15mmHg)		
- 2-Methyl-5-nitrophenol	$\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	153.14	5428-54-6	116~118	106~108(9.5mmHg)		
- 3-Methyl-2-nitrophenol	$\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	153.14	4920-77-8	38~41	125(22mmHg)		
- 4-Methyl-2-nitrophenol	$\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	153.14	119-33-5	30.0~36.5		1.24(38.6/)	
- 4-Methyl-3-nitrophenol	$\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	153.14	2042-14-0	77			
- 5-Methyl-2-nitrophenol	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2\text{OH}$	153.14	700-38-9	54~56			
- 3-Methyl-4-nitrophenol	$\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	153.14	2581-34-2	128~130		1.863(24/4)	0.5%
- 2,4-Dinitrophenol	$(\text{NO}_2)_2\text{C}_6\text{H}_3\text{OH}$	184.11	51-28-5	113~114			難溶
- 2,5-Dinitrophenol	$(\text{NO}_2)_2\text{C}_6\text{H}_3\text{OH}$	184.11	329-71-5	105~113		1.645	難溶
- 2,6-Dinitrophenol	$(\text{NO}_2)_2\text{C}_6\text{H}_3\text{OH}$	184.11	573-56-8	64	昇華		難溶
- 2,6-Dinitro-p-cresol	$\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2(\text{OH})$	198.14	609-93-8	85			難溶
- 4,6-Dinitro-p-cresol	$(\text{NO}_2)_2\text{C}_6\text{H}_3(\text{CH}_3)(\text{OH})$	198.14	534-52-1	86.5			難溶
- Picric acid	$\text{HO}_3\text{C}_6\text{H}_2(\text{NO}_2)_3$	229.11	88-89-1	121~123		1.767(19/)	不溶(冷)微溶(湯)
- 1-Naphthol (α -)	$\text{C}_{10}\text{H}_7\text{OH}$	144.17	90-15-3	95~97	昇華	1.099(99/4)	難溶
- 2-Naphthol (β -)	$\text{C}_{10}\text{H}_7\text{OH}$	144.17	135-19-3	121~123	278~288	1.217	
5-Methyl-2-isopropyl-1-phenol	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}(\text{CH}_3)_2\text{OH}$	150.22	89-83-8	49~52	285~286		
3-Methyl-4-isopropyl phenol	$\text{C}_6\text{H}_4(\text{CH}_3)_2\text{C}_6\text{H}_5\text{OH}$	150.22	3228-02-2	110~113			
Hydroxyhydroquinone	$\text{C}_6\text{H}_2(\text{OH})_2$	126.11	533-73-3	141			
o-sec-Butylphenol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}_6\text{H}_4\text{OH}$	150.22	89-72-5			0.983(20/4)	易溶
p-sec-Butylphenol	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}_6\text{H}_4\text{OH}$	150.22	99-71-8				
o-tert-Butylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{OH}$	150.22	88-18-6			0.983(20/20)	
m-tert-Butylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{OH}$	150.22	585-34-2				
p-tert-Butylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{OH}$	150.22	98-54-4	96~101			
2-tert-Butyl-4-methylphenol	$\text{C}_{11}\text{H}_{14}\text{O}$	164.25	2409-55-4	52			
2-tert-Butyl-5-methylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)\text{OH}$	164.25	88-60-8				
2-tert-Butyl-6-methylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	164.25	2219-82-1				
2,6-Di-tert-butyl-p-cresol (BHT)	$\text{CH}_3\text{C}_6\text{H}_2[(\text{CH}_3)_3\text{C}]_2\text{OH}$	220.35	128-37-0	71	265	1.048(25/4)	
4,6-Di-tert-butyl-m-cresol	$[\text{C}(\text{CH}_3)_2]_2\text{C}_6\text{H}_3(\text{CH}_3)_2\text{OH}$	220.35	497-39-2	62			
2,6-Di-tert-butyl-p-ethylphenol	$\text{C}_6\text{H}_3\text{C}_2\text{H}_5[(\text{CH}_3)_3\text{C}]_2\text{OH}$	234.38	4130-42-1	45			
2,4-Di-tert-butylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_3\text{OH}$	206.33	96-76-4	56			
2,6-Di-tert-butylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_3\text{OH}$	206.33	128-39-2	33~38	253		0.00000597%
2,6-Di-sec-butylphenol	$[\text{C}_4\text{H}_9\text{CH}(\text{CH}_3)]_2\text{C}_6\text{H}_3\text{OH}$	206.33	5510-99-6				
3,5-Di-tert-butylphenol	$[(\text{CH}_3)_3\text{C}]_2\text{C}_6\text{H}_3\text{OH}$	206.33	1138-52-9				
- 2,4,6-Tri-tert-butylphenol	$(\text{CH}_3)_3\text{C}_3\text{C}_6\text{H}_2\text{OH}$	282.44	732-26-3	129~132	277		
- p-tert-Octylphenol	$(\text{CH}_3)_3\text{CC}_6\text{H}_4\text{C}(\text{CH}_3)_2\text{C}_8\text{H}_{17}\text{OH}$	206.33	140-66-9	78~84			
Dichlorodihydroxy-methoxybenzene	$\text{C}_6\text{H}_2\text{Cl}_2\text{O}_2$	209.03	75562-93-5				
* Dichloro-1,2-dihydroxy-3-methoxybenzene	$\text{C}_6\text{H}_2\text{Cl}_2\text{O}_3$	209.03					

アルコール

表1. 微量有機化合物の一覧表

No. 9

化合物名 (英語名)	化学式	分子重量	Cas番号	融点	沸点	比重	水への溶解性
** Methanol	CH ₃ OH	32.04	67-56-1	-96	64.65	0.7928(20/4)	無限
- 2-Chloroethanol (Ethylene chlorohydrin)	ClCH ₂ CH ₂ OH	80.52	107-07-3	-67.5	128.6	1.205(20/20)	無限
- 2-Bromoethanol	BrCH ₂ CH ₂ OH	124.97	540-51-2	液体	148(54.5mmHg)分解	1.75	無限
# 2,2-Dichloroethanol	Cl ₂ CHCH ₂ OH	114.96	598-38-9	液体	146	1.145(15/)	難溶
2,2,2-Trichloroethanol	CCl ₃ CH ₂ OH	149.42	115-20-8	17.8	150(765mmHg)	1.560(20/4)	微溶
1-Chloro-2-propanol	ClCH ₂ CH(OH)CH ₃	94.54	127-00-4	液体	126.7	1.111(20/20)	溶解
3-Chloro-1-propanol	ClCH ₂ CH ₂ CH ₂ OH	94.54	627-30-5	油	160~162	1.131(20/20)	溶解
1-Bromo-2-propanol	BrCH ₂ CH(OH)CH ₃	138.99	19686-73-8	液体	144~148	1.57~1.60	溶解
3-Bromo-1-propanol	BrCH ₂ CH ₂ CH ₂ OH	138.99	627-18-9	液体	60~61(1mmHg)	1.60	溶解
1,3-Dichloro-2-propanol	(ClCH ₂) ₂ CHOH	128.99	96-23-1	<-20	174~175.8	1.367(20/4)	11%(冷)16%(沸)
- 2,3-Dichloro-1-propanol	ClCH ₂ CHClCH ₂ OH	128.99	616-23-9	液体	182	1.353(20/4)	14.5%
1,3-Dibromo-2-propanol	(BrCH ₂) ₂ CHOH	217.89	96-21-9	液体	214.8	2.120(25/)	不溶
2,3-Dibromo-2-propanol	BrCH ₂ CHBrCH ₂ OH	217.89	96-13-9	液体	99(10mmHg)	2.136(20/4)	難溶
** Trichloro-2-propanol	CHCl ₂ CH(OH)CH ₂ Cl	163.43	76-00-6	50	161~162		
3,3,3-Trichloropropanol	C ₃ H ₅ Cl ₃ O	163.43	64667-32-9				
- n-Butanol	CH ₃ (CH ₂) ₃ OH	74.12	71-36-3	-89	117.5	0.809(20/4)	7.36%
- sec-Butanol	CH ₃ CH ₂ CHOHCH ₃	74.12	5892-23-6	-100	99.5	0.811(15/4)	12.5%
- tert-Butanol (2-Methyl-2-propanol)	(CH ₃) ₃ COH	74.12	75-65-0	24.30~28.45	82.20~82.60	0.78581(20/)	
4-Chloro-1-butanol	HO(CH ₂) ₃ Cl	108.57	928-51-8	97	93~103(30mmHg)	1.089(20/4)	0.835%
- 1,1,1-Trichloro-2-methyl-2-propanol	Cl ₃ CC(CH ₃) ₂ OH	177.46	6001-64-5	-78.5	166.4	0.816(20/4)	難溶
# 1-Pentanol (n-Amyl alcohol)	CH ₃ (CH ₂) ₄ OH	88.15	71-41-0	溶解	138.0	0.807(25/4)	4.2%(20°C)
# 2-Pentanol (sec-Amyl alcohol)	CH ₃ (CH ₂) ₃ CHOHCH ₃	88.15	6032-29-7	液体	119	0.821(20/4)	溶解
# 3-Pentanol	CH ₃ CH ₂ CH(OH)CH ₂ CH ₃	88.15	584-02-1	液体	116	0.823(20/4)	0.1%(10°C)
- 1-Heptanol	CH ₃ (CH ₂) ₆ OH	116.20	111-70-6	-34.6	176	0.818(20/4)	不溶
- 2-Heptanol	CH ₃ (CH ₂) ₅ CHOHCH ₃	116.20	543-49-7	液体	157	0.820(20/4)	
- 4-Heptanol	[CH ₃ (CH ₂) ₃] ₂ CHOH	116.20	589-55-9	-37.2	156	0.825(20/4)	
- 1-Octanol	CH ₃ (CH ₂) ₇ OH	130.23	111-87-5	-14	195	0.819(20/4)	微溶
- 2-Octanol (sec-Octyl alcohol)	CH ₃ (CH ₂) ₆ CHOHCH ₃	130.23	123-96-6	-38.6	179	0.830(20/)	0.13%(25°C)
- 1-Decanol	CH ₃ (CH ₂) ₉ OH	158.29	112-30-1	7	232.9	0.820~0.825(20/)	微溶
- 2-Decanol	CH ₃ (CH ₂) ₈ CHOHCH ₃	158.29	1120-06-5	-6~2.80	208~209		
- 1-Tridecyl alcohol	CH ₃ (CH ₂) ₁₂ OH	200.37	112-70-9	30.5	155(13mmHg)		
- 2-Tridecyl alcohol	CH ₃ (CH ₂) ₁₁ CHOHCH ₃	200.37	1653-31-2				
# 1-Ethylcyclobutanol	C ₄ H ₉ (OH)CH ₂ CH ₃	96.13	20434-30-4	液体	59~62		
2-Ethylcyclobutanol	C ₄ H ₉ (OH)CH ₂ CH ₃	96.13	35301-43-0	液体	166~167	1.130(20/4)	無限
3-Ethylcyclobutanol	C ₄ H ₉ (OH)CH ₂ CH ₃	96.13	69647-60-5	液体	171~172	1.116(20/20)	無限
cis-2-Ethylcyclobutanol	C ₄ H ₉ (OH)CH ₂ CH ₃	96.13	57313-97-0	液体	187~189	0.900(20/4)	5%
trans-2-Ethylcyclobutanol	C ₄ H ₉ (OH)CH ₂ CH ₃	96.13	57313-96-9	液体	192	1.038(20/20)	無限
- 2-Methoxyethanol	CH ₃ OCH ₂ CH ₂ OH	76.10	109-86-4	液体	124	0.967(20/20)	難溶
- 2-Ethoxyethanol	C ₂ H ₅ OCH ₂ CH ₂ OH	90.12	110-80-5	-70	135	0.930(20/4)	無限
- 3-Methoxy-1-butanol	CH ₃ CH(OCH ₃)CH ₂ CH ₂ OH	104.15	2517-43-3	液体	166~167	1.130(20/4)	無限
+ 2,3-Epoxy-1-propanol	C ₃ H ₆ O ₂	74.08	556-52-5	液体	171.85	1.116(20/20)	無限
- Ethylene glycol (1,2-Ethanediol)	CH ₂ OHCH ₂ OH	62.07	107-21-1	-11.2~-12.6	197.85	1.261(20/20)	5%
- 2-Butoxyethanol	CH ₃ (CH ₂) ₃ OCH ₂ CH ₂ OH	118.18	111-76-2	液体	187~189	1.038(20/20)	無限
+ Propylene glycol	CH ₃ CH(OH)CH ₂ OH	76.10	57-55-6	-59.5	192	1.003(20/4)	易溶
1,2-Butanediol	CH ₃ CH ₂ CH(OH)CH ₂ OH	90.12	26171-83-5	液体	204~207.5	1.008(20/4)	易溶
- 1,3-Butanediol	CH ₃ (OH)CH ₂ CH(OH)CH ₃	90.12	107-88-0	<-50			

表 1. 微量有機化合物の一覧表

No. 10

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
- 1,4-Butanediol	CH ₂ (OH)CH ₂ CH ₂ CH ₂ OH	90.12	110-63-4	19.5~20.1	229.2~235	1.019(20/4)	無限
- 2-Methyl-2,4-pentanediol	(CH ₃) ₂ C(OH)CH ₂ CH(OH)CH ₃	118.18	107-41-5			0.922(20/4)	
- 3-Methyl-1,5-pentanediol	HOCH ₂ CH ₂ (CH ₃)CHCH ₂ CH ₂ OH	118.18	4457-71-0			0.976(20/4)	
# Allyl alcohol(2-Propen-1-ol)	CH ₂ =CHCH ₂ OH	58.08	107-18-6	-129	96.9	0.853(20/20)	1.0%以上
# 6-Chlorovaniillyl alcohol	Cl(CH ₃ O)C ₆ H ₄ (OH)CH ₂ OH	188.62	18268-77-4				
# Dichlorovaniillyl alcohol	Cl ₂ (CH ₃ O)C ₆ H ₃ (OH)CH ₂ OH	223.07					
# Trichlorovaniillyl alcohol	Cl ₃ (CH ₃ O)C ₆ (OH)CH ₂ OH	257.52					
# 1-(Dichloro-3,5-dimethoxy-4-hydroxyphenyl)-1-ethanol	Cl ₂ (CH ₃ O) ₂ C ₆ (OH)CH(OH)CH ₃	267.12					
* Dichlorodiferyl alcohol	C ₁₀ H ₁₁ O ₃ Cl ₂	249.09					
# Dichlorodihydroconiferyl alcohol	Cl ₂ (CH ₃ O)C ₆ H ₄ (OH)CH ₂ CH ₂ OH	237.09					
** Trichlorodihydroconiferyl alcohol	Cl ₃ (CH ₃ O)C ₆ (OH)CH ₂ CH ₂ OH	281.525					
# Betuligenol	C ₃₀ H ₄₈ (OH)CH ₂ CH ₂ CH(OH)CH ₃	166.22	501-96-2				
# Borneol(1-)	C ₁₀ H ₁₈ O	154.25	507-70-0	197~207.2	212	1.011	不溶
# 1- α -Terpineol	C ₁₀ H ₁₈ O	154.25	464-45-9	207.2	210(779mmHg)	1.02	不溶
# 1- β -Terpineol	C ₁₀ H ₁₈ O	154.25	98-55-5	37	218	0.934(20/4)	不溶
# β -Sitosterol	C ₂₇ H ₄₈ O	154.25	10482-56-1	32	210	0.923(15/4)	
# Lupeol	C ₃₀ H ₅₀ O	414.72	83-46-5	140			
#	C ₃₀ H ₅₀ O	426.7	545-47-1	216~217			
# Betulinol	C ₃₀ H ₅₀ O ₂	442.73	473-98-3				
- Benzyl alcohol	C ₆ H ₅ CH ₂ OH	108.14	100-51-6	-15.3	204.7~205.4	1.048(20/20)	4%
# o-Chlorobenzyl alcohol	ClC ₆ H ₄ CH ₂ OH	142.59	17849-368-6	69~72			
# m-Chlorobenzyl alcohol	ClC ₆ H ₄ CH ₂ OH	142.59	873-63-2				
# p-Chlorobenzyl alcohol	ClC ₆ H ₄ CH ₂ OH	142.59	873-76-7	70~74	234		
# Chlorocymen-8-ol	ClCH ₃ C ₆ H ₄ C(CH ₃) ₂ OH	185.68					
# Dichlorocymen-8-ol	Cl ₂ CH ₃ C ₆ H ₃ C(CH ₃) ₂ OH	220.13					
# Dichlorodehydroabietyl							
# Arabinose	C ₅ H ₁₀ O ₅	150.13	147-81-9	157~160			100%
* D-Arabinose	CH ₂ (CHOH) ₄ O	150.13	10323-20-3	β 159			易溶
* L-Arabinose	CH ₂ (CHOH) ₄ O	150.13	5328-37-0	α 158 β 160			60%
* D(-)-Arabinose	CH ₂ (CHOH) ₄ O	150.13	28697-53-2	153~161			
* L(+)-Arabinose	CH ₂ (CHOH) ₄ O	150.13	87-72-9	156~160			60%
** Xylose	C ₅ H ₁₀ O ₅	150.13	25990-60-70	144~154			
* D-Xylose	OCH ₂ (CHOH) ₃ CHOH	150.13	58-86-6	144~145			117%(23)
* L-Xylose	OCH ₂ (CHOH) ₃ CHOH	150.13	609-06-3				
** Glucose	C ₆ H ₁₂ O ₆	180.16	50-99-7	146	> 200	1.544(25/4)	81.7%
D-Glucose	CHO(CHOH) ₄ CH ₂ OH	180.16	50-99-7	α 146			易溶
L-Glucose	CHO(CHOH) ₄ CH ₂ OH	180.16	921-60-8				
DL-Glucose	CHO(CHOH) ₄ CH ₂ OH	180.16	58367-01-4				
** Mannose	C ₆ H ₁₂ O ₆	180.16	31103-86-3				
D-Mannose	HOCH ₂ CH(CHOH) ₃ CHOH	180.16	3458-28-4	α 133 β 132			248%(17°C)
L-Mannose	HOCH ₂ CH(CHOH) ₃ CHOH	180.16	10030-80-5				
Galactose	C ₆ H ₁₂ O ₆	180.16	26566-61-0				
# D-Galactose	CHO(CHOH) ₄ CH ₂ OH(4H ₂ O)	180.16	59-23-4	165.5(無水物)			10.3%

表 1. 微量有機化合物の一覧表

No. 11

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
アルデヒド							
** Glyoxal	(CHO) ₂	58.04	107-22-2	15	51(776mmHg)	1.272(20/4)	溶解
- Formaldehyde(Formalin)	HCHO	30.03	50-00-0	-118~-92	96	1.081(25/25)	溶解
** Acetaldehyde	CH ₃ CHO	44.05	75-07-0	-123.5	20.2	0.788(16/4)	溶解
** Chloroacetaldehyde (40% in water)	ClCH ₂ CHO	78.50	107-20-0	液体	85	1.215(20/4)	
* Dichloroacetaldehyde, monomer	Cl ₂ CHCHO·H ₂ O	112.94	79-02-7	56	90		
Trichloroacetaldehyde	Cl ₃ CCHO	147.40	75-87-6	-57.5	97.8	1.510(20/4)	660%
Trichloroacetaldehyde-monohydrate	Cl ₃ CCHO·H ₂ O	165.42	302-17-0	51.6~57	96~98	1.908(20/4)	474%
Tribromoacetaldehyde(Bromal)	Br ₃ CCHO	280.74	115-17-3	液体	174	2.66(25/4)	
- Propanal(Propionaldehyde)	CH ₃ CH ₂ CHO	58.08	123-38-6	-81~-80.05	47.93	0.815(20/4)	16.15%
n-Butyric aldehyde(n-Butyraldehyde)	CH ₃ (CH ₂) ₂ CHO	72.11	123-72-8	-99	75.7	0.802(20/4)	3.7%
iso-Butyric aldehyde	(CH ₃) ₂ CHCHO	72.11	78-84-2		65	0.79	
n-Valeraldehyde	CH ₃ (CH ₂) ₃ CHO	86.13	110-62-3	-91.5	103.7	0.813(20/4)	微溶
iso-Valeraldehyde	(CH ₃) ₂ CHCH ₂ CHO	86.13	590-86-3			0.80	
- Acrolein	CH ₂ =CHCHO	56.06	107-02-8	-86.95~-68	52.69~53	0.838(20/)	53%
2,2-Dichloropropanal	C ₃ H ₄ Cl ₂ O	126.98	27313-32-2	47~53	68~83	1.248(20/)	
# 2,3-Dichloropropanal	CH ₂ Cl ₂ CHCHO	126.98	10140-89-3		73(50.0mmHg)	1.37~1.40(20/)	
3,3-Dichloropropanal	C ₃ H ₄ Cl ₂ O	126.98	14538-09-1		43~44(10mmHg)	1.35790(20/)	
** 2-Chloropropenal	CH ₃ C(Cl)CHO	90.52	683-51-2	37~38	109(759mmHg)	1.199~1.21(20/)	可溶
+ Butenal(Crotonaldehyde)	CH ₃ CH=CHCHO	70.09	123-73-9	-69(trans-76.6)	104.4	0.855(20/4)	
** Chlorobutenal	CH ₃ CCl=CHCHO	104.54					
** Dichlorobutenal	CH ₃ CCl ₂ CHCHO	138.99					
# Pimara	C ₂₀ H ₃₀ O	286.46	472-39-9				
# Isopimaral	C ₂₀ H ₃₀ O	286.46	1886-63-1				
# Benzaldehyde	C ₆ H ₅ CHO	106.12	100-52-7	-26	178	1.049(20/4)	<0.33%
** o-Chlorobenzaldehyde	ClC ₆ H ₄ CHO	140.57	89-98-5	11	213~214(748mmHg)	1.252~1.254(20/4)	難溶
- m-Chlorobenzaldehyde	ClC ₆ H ₄ CHO	140.57	587-04-2	17~18	213~214	1.241(20/4)	難溶
- p-Chlorobenzaldehyde	ClC ₆ H ₄ CHO	140.57	104-88-1	46~49	213	1.196(61/4)	難溶
** Dichlorobenzaldehyde	C ₆ H ₄ Cl ₂ O	175.01	31155-09-6				
2,3-Dichlorobenzaldehyde	Cl ₂ C ₆ H ₃ CHO	175.01	6334-18-5	62			
2,4-Dichlorobenzaldehyde	Cl ₂ C ₆ H ₃ CHO	175.01	874-42-0	69~73			
2,5-Dichlorobenzaldehyde	Cl ₂ C ₆ H ₃ CHO	175.01	6361-23-5	54~59	230~233		
2,6-Dichlorobenzaldehyde	Cl ₂ C ₆ H ₃ CHO	175.01	83-38-5	71			
3,4-Dichlorobenzaldehyde	Cl ₂ C ₆ H ₃ CHO	175.01	6287-38-3	40~44			
3,5-Dichlorobenzaldehyde	Cl ₂ C ₆ H ₃ CHO	175.01	10203-08-4	60~65	215~222(7mmHg)		
# Ethylbenzaldehyde	CH ₃ CH ₂ CH ₂ CHO	134.18	4748-78-1			1.00	
** Furfural	C ₄ H ₃ OCHO	96.09	98-01-1	-36.5	162	1.159(20/4)	9.1%
# Dichloro-3-formyl-thiophene	Cl ₂ C ₄ HSCHO	181.05					
# Trichloro-3-formyl-thiophene	Cl ₃ C ₄ SCHO	215.5					
Trichloro-2-formylthiophene	C ₄ HCl ₃ SO	215.5	66729-79-1				
** 3,5-Dichloro-4-hydroxybenzaldehyde	Cl ₂ C ₆ H ₃ (OH)CHO	191.01					
# Chlorodihydroxybenzaldehyde	ClC ₆ H ₄ (OH) ₂ CHO	172.57					
# Dichlorodihydroxybenzaldehyde	Cl ₂ C ₆ H ₂ (OH) ₂ CHO	207.02					
# Vanillin	CH ₃ OC ₆ H ₄ (OH)CHO	152.15	148-53-8	80.5~83.5	285(昇華)	1.056	0.9%
# Chlorovanillin	C ₆ H ₇ ClO ₃	186.59					
** 2-Chlorovanillin	Cl(CH ₃ O)C ₆ H ₄ (OH)CHO	186.59	82668-20-0				

表 1. 微量有機化合物の一覧表

No. 12

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
5-Chlorovanillin	Cl(CH ₃ O)C ₆ H ₄ (OH)CHO	186.59	19463-48-0				
6-Chlorovanillin	Cl(CH ₃ O)C ₆ H ₄ (OH)CHO	186.59	18268-76-3				
Dichlorovanillin	C ₈ H ₆ Cl ₂ O ₃	221.04	94650-95-0				
2,5-Dichlorovanillin	Cl ₂ (CH ₃ O)C ₆ H ₃ (OH)CHO	221.04	140642-60-0				
2,6-Dichlorovanillin	Cl ₂ (CH ₃ O)C ₆ H ₃ (OH)CHO	221.04	108545-01-3				
5,6-Dichlorovanillin	Cl ₂ (CH ₃ O)C ₆ H ₃ (OH)CHO	221.04	18268-69-4				
Trichlorovanillin	Cl ₃ (CH ₃ O)C ₆ H ₂ (OH)CHO	255.49	119464-51-6				
Chloromethoxydihydroxybenzaldehyde	Cl(CH ₃ O)C ₆ H ₃ (OH) ₂ CHO	202.60					
Chlorosyringaldehyde	Cl(CH ₃ O) ₂ C ₆ H ₃ (OH)CHO	216.63					
2-Chlorosyringaldehyde	Cl(CH ₃ O) ₂ C ₆ H ₃ (OH)CHO	216.63	76341-69-0				
Dichlorosyringaldehyde	Cl ₂ (CH ₃ O) ₂ C ₆ H ₂ (OH)CHO	251.07	76330-06-8				
2,6-Dichlorosyringaldehyde	Cl ₂ (CH ₃ O) ₂ C ₆ H ₂ (OH)CHO	251.07					
Chloroprotocatechualdehyde	C ₇ H ₅ ClO ₃	172.56					
2-Chloroprotocatechualdehyde	C ₇ H ₄ ClO ₃	172.56	32864-11-2				
6-Chloroprotocatechualdehyde	C ₇ H ₄ ClO ₃	172.56	37686-56-9				
Dichloroprotocatechualdehyde	C ₇ H ₃ Cl ₂ O ₃	207					
ケトン							
Bromoacetone	CH ₃ COCH ₂ Br	136.98	598-31-2	液体	136.5(725mmHg)	1.622(16/)	難溶
Chloroacetone	CH ₃ COCH ₂ Cl	92.52	78-95-5	-44	119~120	1.155(20/4)	溶解
Dichloroacetone	C ₃ H ₄ Cl ₂ O	126.97	30605-38-0				
1,1-Dichloroacetone	CH ₃ COCHCl ₂	126.97	513-88-2		117~120	1.236(21/)	微溶
1,3-Dichloroacetone	ClCH ₂ COCH ₂ Cl	126.97	534-07-6	39~45	172.5~173	1.383(46/4)	溶解
Trichloroacetone	C ₃ H ₃ Cl ₃ O	161.41	72497-18-8				
1,1,1-Trichloroacetone	CH ₃ COCCl ₃	161.41	918-00-3		134~135	1.435	
1,1,3-Trichloroacetone	Cl ₂ CHCOCH ₂ Cl	161.41	921-03-9	13~15	172°C	1.508	
Tetrachloroacetone	Cl ₃ CCOCH ₂ Cl	195.88		液体	180(718mmHg)	1.624(15/4)	
α, α, α -Tetrachloroacetone	Cl ₃ CCOCH ₂ Cl	195.88	16995-35-0	液体	180(718mmHg)	1.624(15/4)	
1,1,1,3-Tetrachloroacetone	Cl ₃ CCOCH ₂ Cl	195.88	632-21-3		118~120(100mmHg)	1.624(20/)	
1,1,3,3-Tetrachloroacetone	Cl ₂ CHCOCHCl ₂	230.33	1768-31-6	2.10	184	1.50(20/)	
Pentachloroacetone	Cl ₃ CCOCHCl ₂	230.33	1768-31-6		191	1.66(20/)	
Hexachloroacetone	CCl ₃ COCCl ₃	264.75	116-16-5			1.742(20/4)	
2-Butanone(Ethylmethylketone)	CH ₃ CH ₂ COCH ₃	72.11	78-93-3	-86.6	79.6	0.807(20/20)	35.5%
Chlorobutanone	C ₄ H ₇ OC1	106.55					
Dichlorobutanone	C ₄ H ₆ OC1 ₂	140.99					
Trichlorobutanone	C ₄ H ₅ OC1 ₃	175.43					
3-Hydroxy-3-methoxy-2-butanone	CH ₃ COOCH ₂ (OCH ₃)CH ₃	118.14					
Methylpentanone	C ₆ H ₁₂ O	100.16	63072-44-6				
2-Methyl-3-pentanone	CH ₃ CH(CH ₃)COCH ₂ CH ₃	100.16					
3-Methyl-2-pentanone	CH ₃ CH ₂ CH(CH ₃)COCH ₃	100.16	565-61-7				
4-Methyl-2-pentanone	(CH ₃) ₂ CHCH ₂ COCH ₃	100.16	108-10-1	-83.5	116.7	0.7978(20/4)	
4-Methyl-3-pentanone	(CH ₃) ₂ CHCOCH ₂ CH ₃	100.16					
2,4-Dimethyl-3-pentanone	CH ₃ CH(CH ₃)COCH(CH ₃)CH ₃	114.19	565-80-0			0.805(20/4)	
4,4-Dimethyl-2-pentanone	(CH ₃) ₃ COCH ₂ COCH ₃	114.19	590-50-1			0.804(20/4)	
4-Hydroxy-4-methyl-2-pentanone	CH ₃ COCH ₂ (OH)(CH ₃)CH ₃	104.15					
Chloropentanone	C ₅ H ₉ OC1	120.58					

表1. 微量有機化合物の一覧表

No. 13

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
1-Chloro-3-pentanone	C ₅ H ₉ ClO	120.58	32830-97-0		63(25mmHg)	1.0458(20/)	
5-Chloro-2-pentanone	Cl(CH ₂) ₃ COCH ₃	120.58	5891-21-4		106(110mmHg)	1.0523(20/)	
Dichloropentanone	C ₅ H ₇ OCl ₂	155.03					
Trichlorocyclopropanone	C ₃ HOC1 ₃	159.4					
Chlorocyclopropanone	C ₃ HClO	88.50					
Dichlorocyclopropanone	C ₃ Cl ₂ O	122.95					
Hydroxy-methoxyacetophenone	C ₈ H ₉ O ₃	166.18	20434-10-0				
4-Hydroxy-3-methoxyacetophenone	CH ₃ OC ₆ H ₃ (OH)COCH ₃	166.18	120519-66-6				
Dichloroacetosyringone	Cl ₂ (CH ₃ O) ₂ C ₆ (OH)COCH ₃	265.09					
2,6-Dichloroacetosyringone	Cl ₂ (CH ₃ O) ₂ C ₆ (OH)COCH ₃	265.09					
Trichloroacetosyringone	Cl ₂ (CH ₃ O) ₂ C ₆ (OH)COCH ₂ Cl	299.55					
Dichloropropyl catechol	Cl ₂ (CH ₃ CH ₂) ₂ C ₆ H(OH) ₂	221.09					
Chloro-3,4-dihydroxypropionophenone	ClC ₆ H ₂ (OH) ₂ COCH ₂ CH ₃	200.62					
Dichloro-3,4-dihydroxy-propionophenone	Cl ₂ C ₆ H(OH) ₂ COCH ₂ CH ₃	235.06					
Chloropropionatone	Cl(CH ₃ O)C ₆ H ₂ (OH)COCH ₂ CH ₃	214.66					
1-(Dichloro-3,5-dimethoxy-4-hydroxyphenyl)-2-propanone	Cl ₂ (CH ₃ O) ₂ C ₆ (OH)CH ₂ COCH ₃	279.13					
2-Butanone	CH ₃ COCH ₂ CH ₃	70.09	78-94-4	液体	81.4	0.8459(20/4)	
Cyclobutanone	C ₄ H ₆ O	88.08					
2-Cyclobutanone	C ₄ H ₆ O	88.08	32264-87-2				
Chlorocyclobutanone	C ₄ H ₅ ClO	102.53					
Dichlorocyclobutanone	C ₄ H ₄ Cl ₂ O	136.97					
Trichlorocyclobutanone	C ₄ HOC1 ₃	171.41					
Tetrachlorocyclobutanone	C ₄ Cl ₄ O	205.87	3200-96-2	-1	174~176		
Penphone	C ₈ H ₁₆ O	152.24					
d-Camphor	C ₁₅ H ₂₄ O	152.24	76-22-2	178~179	209(昇華)	0.999(9/9)	0.1%
(-)-Camphor	C ₁₅ H ₂₄ O	152.24	464-48-2				
(+)-Camphor	C ₁₅ H ₂₄ O	152.24	464-49-3	177~182			
(±)-Camphor	C ₁₅ H ₂₄ O	152.24	21368-88-3	174~180			
Epichlorohydrine(Chloromethyl oxirane)	OC1H ₂ CHCl ₂ Cl	92.52	106-89-8	-48~-25.6	117.9	1.182(20/4)	6.58%
1,4-Dioxane	C ₄ H ₈ O ₂	88.11	123-91-1	9~13	100.0~101.6	1.036(20/20)	易溶
Chlorocyclopentene-1,2-dione	ClC ₅ H ₇ (:O) ₂	134.57					
Dichlorocyclopentene-1,2-dione	Cl ₂ C ₅ H ₆ (:O) ₂	166.99					
Trichlorocyclopentene-1,2-dione	Cl ₃ C ₅ H ₅ (:O) ₂	201.44					
Tetrachlorocyclopentene-1,2-dione	Cl ₄ C ₅ H ₄ (:O) ₂	235.88					
Tetrachlorocyclopentene-1,3-dione	Cl ₄ C ₅ H ₄ (:O) ₂	235.88					
Tetrachlorocyclopentene-2,4-dione	C ₅ Cl ₄ O ₂	235.88					
Dichlorobenzoquinone	C ₆ H ₂ Cl ₂ O ₂	176.99	15743-13-2	64~68	148(25~30mmHg)	1.75	
Dichloro-1,2-benzoquinone	Cl ₂ C ₆ H ₂ (:O) ₂	176.99	26912-70-9				
Dichloro-2,3-benzoquinone	Cl ₂ C ₆ H ₂ (:O) ₂	176.99					
Dichloro-2,6-benzoquinone	Cl ₂ C ₆ H ₂ (:O) ₂	176.99	5145-42-6	96~102			
Tetrachloro-1,2-benzoquinone	Cl ₄ C ₆ (:O) ₂	245.88	697-91-6				
1-oxa-6,10,10-trichlorospiro[4,5]dec-6-en-8,9-dione	C ₆ H ₂ O ₃ Cl ₃	269.53					
1-oxa-6,7,10,10-tetrachlorospiro[4,5]dec-6-en-8,9-dione	C ₆ H ₂ O ₃ Cl ₄	303.98					
Acetophenone	C ₆ H ₅ COCH ₃	120.15	98-86-2	20	202	1.024(25/4)	微溶

表 1. 微量有機化合物の一覧表

No. 14

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
# Benzanthracene-7-one	C ₁₇ H ₁₀ O	230.27					
# Fluorenone	C ₁₃ H ₈ O	180.21	486-25-9	80~86	341.5	1.130(99/4)	不溶
2-Acetylthiophene	C ₆ H ₄ S(OCCH ₃)	126.18	88-15-3		213.5	1.168(22/)	
* 3-Acetylthiophene	C ₆ H ₄ S(OCCH ₃)	126.18	1468-83-3	60	208~210(748mmHg)		
* 2-Acetyldichlorothiophene	C ₆ H ₂ Cl ₂ S	195.07					
* 3-Acetyldichlorothiophene	C ₆ H ₂ Cl ₂ S	195.07					
* 2-Acetyltrichlorothiophene	C ₆ H ₂ Cl ₃ S	229.52					
# 3-Acetyltrichlorothiophene	C ₆ H ₂ Cl ₃ S	229.52					
* Dichloropropylthiophene	C ₇ H ₆ Cl ₂ S	209.09					
* 3-Chloro-2-propionylthiophene	C ₇ H ₆ Cl ₂ S	209.09					
** 3-Chloro-4-dichloromethyl-5-hydroxy-2(5H)-furanone (MX)	C ₈ H ₄ O ₃ Cl ₃	217.44	77439-76-0				
# 3-Chloro-5-dichloromethylene-2(5H)-furanone	C ₈ H ₂ O ₃ Cl ₃	199.43					
# 4-Chloro-5-dichloromethylene-2(5H)-furanone	C ₈ H ₂ O ₃ Cl ₃	199.43					
# 3,4-Dichloro-5-dichloromethylene-2(5H)-furanone	C ₈ O ₃ Cl ₄	233.88					
# 3,4-Dichloro-5-dichloromethyl-5-hydroxy-2(5H)-furanone	C ₈ H ₂ O ₃ Cl ₄	251.90					
1,2-Pyrone	C ₅ H ₄ O ₂	96.09	504-31-4	5	206~207	1.1880(22/4)	無限 易溶
1,4-Pyrone	C ₅ H ₄ O ₂	96.09	108-97-4	32.5	215(742mmHg)		
# Chloropyrone	C ₅ H ₄ ClO ₂	130.54					
# Dichloropyrone	C ₅ H ₂ Cl ₂ O ₂	164.99					
# Trichloropyrone	C ₅ HCl ₃ O ₂	199.43					
# Tetrachloro-2-pyrone	C ₅ Cl ₄ O ₂	233.88					
# Tetrachloro-α-pyrone	C ₅ Cl ₄ O ₂	233.88	10269-62-2				
エーテル							
- 2-Chloroethyl vinyl ether	ClCH ₂ CH ₂ OCCH=CH ₂	106.55	110-75-8	液体	109(740mmHg)		
# 5-Pentyl-oxy-2-pentene	CH ₃ CH ₂ CH(CH ₂) ₂ O(CH ₂) ₅ CH ₃	156.27					
- Diphenyl ether (Phenyl ether)	C ₆ H ₅ OC ₆ H ₅	170.21	101-84-8	26~28	259.3	1.148(20/)	殆不溶
+ Dibenzyl ether	(C ₆ H ₅ CH ₂) ₂ O	198.26	103-50-4	3.6	296	1.046(20/4)	
エステル							
- Methyl formate	HCOCCH ₃	60.05	107-31-3	-99.0	31.5	0.975(20/4)	21%
- Ethyl formate	HCOC ₂ H ₅	74.08	109-94-4	-80.5	54.1	0.921(20/4)	11%
n-Propyl formate	HCOCCH ₂ CH ₂ CH ₃	88.11	110-74-7	-92.9	81.2	0.885(20/4)	
Isopropyl formate	HCOC(CH ₃) ₂	88.11	625-55-8		66.50~71.00	0.87(20/)	
- n-Butyl formate	HCOC(CH ₂) ₃ CH ₃	102.13	592-84-7			0.894(20/4)	1.01%
- Isobutyl formate	HCOCCH ₂ CH(CH ₃) ₂	102.13	542-55-2	-95.8	97.7	0.885(20/4)	
Propyl acetate	CH ₃ COOCH ₂ CH ₂ CH ₃	102.13	109-60-4	-95.0	101.6		
Isopropyl acetate	CH ₃ COOCH(CH ₃) ₂	102.13	108-21-4		89.4~89.5		
Allyl formate	HCOCCH=CH ₂	86.09	1838-59-1	液体	83~84	0.948(18/)	
Butyl acetate	CH ₃ COO(CH ₂) ₃ CH ₃	116.16	123-86-4		126.3	0.883(20/20)	
s-Butyl acetate	CH ₃ COOCH ₂ CH(CH ₃) ₂	116.16	105-46-4	-98.9	112.2		
t-Butyl acetate	CH ₃ COOC(CH ₃) ₃	116.16	540-88-5		97.8		
Chloroacetic acid methyl ester	ClCH ₂ COOCH ₃	108.52	96-34-4		130	1.24	
Chloroacetic acid ethyl ester	ClCH ₂ COOCH ₂ CH ₃	122.55	105-39-5		143	1.15	
** Dichloroacetic acid methyl ester	Cl ₂ CHCOOCH ₃	142.97	116-54-1		143	1.38	
** Dichloroacetic acid ethyl ester	Cl ₂ CHCOOCH ₂ CH ₃	157	535-15-9				

表 1. 微量有機化合物の一覧表

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
Trichloroacetic acid methyl ester	$\text{Cl}_3\text{CCOOCH}_3$	177.41	598-99-2		154	1.49	
Trichloroacetic acid ethyl ester	$\text{Cl}_3\text{CCOOCH}_2\text{CH}_3$	191.44	515-84-4			1.39	
Methyl acrylate	$\text{CH}_2=\text{CHCOOCH}_3$	86.09	96-33-3	<-75	79.6~80.3	0.959(20/4)	
Ethyl acrylate	$\text{CH}_2=\text{CHCOOC}_2\text{H}_5$	100.12	140-88-5	-71.2	99.3~99.7	0.924(20/4)	
n-butyl acrylate	$\text{CH}_2=\text{CHCOO}(\text{CH}_2)_3\text{CH}_3$	128.17	141-32-2	-64.6	146.2~148	0.899(20/4)	
tert-butyl acrylate	$\text{CH}_2=\text{CHCOOC}(\text{CH}_3)_3$	128.17	1663-39-4			0.878(20/4)	
2-Ethylhexyl acrylate	$\text{CH}_2=\text{CHCOOCH}_2(\text{C}_2\text{H}_5)_2\text{CH}(\text{CH}_2)_3\text{CH}_3$	184.28	103-11-7			0.885(20/4)	
Methyl methacrylate	$\text{CH}_2=\text{C}(\text{CH}_3)\text{COOCH}_3$	100.12	80-62-6			0.945(20/4)	
Ethyl methacrylate	$\text{CH}_2=\text{C}(\text{CH}_3)\text{COOC}_2\text{H}_5$	114.14	97-63-2			0.915(20/4)	
n-Butyl methacrylate	$\text{CH}_2=\text{C}(\text{CH}_3)\text{COO}(\text{CH}_2)_3\text{CH}_3$	142.20	97-88-1			0.897(20/4)	
Isobutyl methacrylate	$\text{CH}_2=\text{C}(\text{CH}_3)\text{COOCH}_2\text{CH}(\text{CH}_3)_2$	142.20	97-86-9			0.886(20/4)	
tert-Butyl methacrylate	$\text{C}_4\text{H}_9\text{O}_2$	142.20	585-07-9			0.877(20/4)	
Glycidyl methacrylate	$\text{OCH}_2\text{CHCH}_2\text{OCO}(\text{CH}_3)_2\text{C}(\text{CH}_3)_2$	142.15	106-91-2			1.079(20/4)	
Methylbenzoate	$\text{C}_6\text{H}_5\text{COOCH}_3$	136.15	93-58-3	-12.5	199.5	1.094(15/4)	不溶
Chlorobenzoate	$\text{ClC}_6\text{H}_4\text{COOCH}_3$	170.59					
1-Acetoxy-2-methoxyethane	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OCH}_3$	118.13	110-49-6			1.008(20/4)	
1-Acetoxy-2-ethoxyethane	$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OC}_2\text{H}_5$	132.16	111-15-9			0.975(20/4)	
Acetic acid 3-methoxybutyl ester	$\text{CH}_3\text{COO}(\text{CH}_2)_2\text{CH}(\text{OCH}_3)\text{CH}_3$	146.19	4435-53-4			0.96	
炭化水素							
Dichloromethane	CH_2Cl_2	84.93	75-09-2	-96	40.21~41.6	1.336(20/4)	2%
Dibromomethane	CH_2Br_2	173.84	74-95-3			2.498(20/20)	
Bromochloromethane	BrCH_2Cl	129.38	74-97-5			1.941(20/4)	
Chloroform	CHCl_3	119.38	67-66-3	-63.5	61~62	1.484(20/20)	0.822%
Carbon tetrachloride	CCl_4	153.82	56-23-5	-22.6	76.7	1.592(20/4)	0.08%
Carbon tetrabromide	CBr_4	331.63	558-13-4	α 48.4, β 90.1	189.5	3.42	難溶
Bromodichloromethane	CHBrCl_2	163.83	75-27-4	-57.1	87~90	1.980(20/)	0.322%
Dibromochloromethane	CHBr_2Cl	208.28	124-48-1		116	2.38(20/)	0.105%
Bromoform	CHBr_3	252.73	75-25-2	7.5~8.05	149.6	2.904(15/4)	0.319%
Trichlorofluoromethane	CCl_3F	137.37	75-69-4			1.49	
Nitromethane	CH_3NO_2	61.04	75-52-5	-28.5	101.25	1.133(20/20)	微溶
Chloroethane(Ethyl chloride)	$\text{C}_2\text{H}_5\text{Cl}$	64.51	75-00-3	-138.7	13.1	0.917(6/)	難溶
Bromoethane	$\text{C}_2\text{H}_5\text{Br}$	109.0	74-96-4	-126	38	1.465(20/4)	
1,1-Dichloroethane	CH_3CHCl_2	98.96	75-34-3	-96.7	57~57.3	1.174(20/4)	0.55%(25°C)
1,1-Dibromoethane	CH_3CHBr_2	187.86	557-91-5	液体	109	2.089(20/)	
1,2-Dichloroethane	$\text{CH}_2\text{ClCH}_2\text{Cl}$	98.96	107-06-2	-35.3	83.38~83.7	1.258(17/4)	0.85%~0.87%
1,2-Dibromoethane	$\text{CH}_2\text{BrCH}_2\text{Br}$	187.86	106-93-4	9.5	131.6	2.180(20/)	0.43%(30°C)
1,1,1-Trichloroethane(Methylchloroform)	CH_3CCl_3	133.40	71-55-6	-33.0	73.9~75	1.325(20/4)	不溶
1,1,2-Trichloroethane	$\text{CH}_2\text{ClCHCl}_2$	133.40	79-00-5	-35.5	113.6	1.440(20/4)	0.44%(20°C)
1,1,2-Tribromoethane	$\text{CH}_2\text{BrCHBr}_2$	266.76	78-74-0	-29.2	188	2.579(20/)	
1,1,1,2-Tetrachloroethane	$\text{CCl}_3\text{CH}_2\text{Cl}$	167.85	630-20-6	-68.1	130~131	1.588(20/4)	0.02%
1,1,2,2-Tetrachloroethane	$\text{CHCl}_2\text{CHCl}_2$	167.85	79-34-5	42.5	146.3	1.600(20/4)	不溶
1,1,2,2-Tetrabromoethane	$\text{CHBr}_2\text{CHBr}_2$	345.65	79-27-6	0.1	123.7~243	2.965(20/20)	0.065%(30°C)
Pentachloroethane	$\text{CHCl}_2\text{CCl}_3$	202.29	76-01-7	-29.0	161~162	1.688(15/4)	0.106%(20°C)
Hexachloroethane	CCl_3CCl_3	236.74	67-72-1	182~186	昇華	2.091	不溶
Nitroethane	$\text{C}_2\text{H}_5\text{NO}_2$	75.07	79-24-3	-89.5	114.0	1.052(20/4)	不溶

表 1. 微量有機化合物の一覧表

No. 16

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
- 1,1-Dichloroethylene	CH ₂ :CCl ₂	96.94	75-35-4	液体	34~35	1.250(15/)	
+ cis-1,2-Dichloroethylene	CHCl:CHCl	96.94	156-59-2	-80.5	60.3	1.292(15/)	0.35%
+ trans-1,2-Dichloroethylene	CHCl:CHCl	96.94	156-60-5	-50.0	47.48~48.4	1.255(20/4)	0.63%
- cis-1,2-Dibromoethylene	BrCH:CHBr	185.86	540-49-8	-53	112.5	2.285(18/)	
- trans-1,2-Dibromoethylene	BrCH:CHBr	185.86	540-49-8	-6.5	108	2.267(18/)	
##+ Trichloroethene(Trichloroethylene)	Cl ₂ C:CHCl	131.39	79-01-6	-73	87.2	1.456(25/4)	0.1%(10°C)
##+ Tetrachloroethene(Tetrachloroethylene)	Cl ₂ C:CCl ₂	165.83	127-18-4	-19	121.1	1.622(20/4)	不溶
- 1-Chloropropane	CH ₃ CH ₂ CH ₂ Cl	78.54	540-54-5	-122.8	46.4	0.864~0.892(20/4)	0.27%
- 2-Chloropropane	(CH ₃) ₂ CHCl	78.54	75-29-6	-117.0	36.5	0.868(15/)	0.30%
- 1-Bromopropane	CH ₃ CH ₂ CH ₂ Br	122.99	106-94-5	-110	71	1.353(20/4)	0.25%(20°C)
2-Bromopropane	(CH ₃) ₂ CHBr	122.99	75-26-3	-89.0	59.4	1.313(20/4)	0.32%(20°C)
1,1-Dichloropropane	CH ₃ CHClCH ₂ Cl	112.99	78-99-9	液体	85~87	1.143(10/)	
- 1,2-Dichloropropane	CH ₃ CHClCH ₂ Cl	112.99	78-87-5	液体	96.4~98	1.166(14/)	0.28%(25°C)
1,3-Dichloropropane	ClCH ₂ CH ₂ CH ₂ Cl	112.99	142-28-9	液体	125	1.190(20/4)	0.273%(25°C)
2,2-Dichloropropane	CH ₃ CCl ₂ CH ₃	112.99	594-20-7	-34.6	69.7	1.097(15/15)	
Bromochloropropane	C ₃ H ₇ BrCl	157.44	34652-54-5		143	1.600(20/4)	
1-Bromo-3-chloropropane	BrCH ₂ CH ₂ CH ₂ Cl	157.44	109-70-6		133	1.35	
1,1,2-Trichloropropane	CH ₂ CHClCHCl ₂	147.43	598-77-6		156.9	1.394(20/4)	0.1%以下
- 1,2,3-Trichloropropane	ClCH ₂ CHClCH ₂ Cl	147.43	96-18-4	-14.7	196	2.08~2.11(20/20)	
# - 1,2-Dibromo-3-chloropropane	ClCH ₂ CHBrCH ₂ Br	236.33	96-12-8				
1-Bromo-4-chlorobutane	Br(CH ₂) ₄ Cl	171.46					
1-Bromo-5-chloropentane	Br(CH ₂) ₅ Cl	185.49					
- 1-Nitropropane	CH ₃ CH ₂ CH ₂ NO ₂	89.09	108-03-2	-108	131.6	1.002(20/4)	不溶
- 2-Nitropropane	(CH ₃) ₂ CHNO ₂	89.09	79-46-9	-93	120.3	0.994(20/4)	不溶
- 3-Chloro-1-propene(Allyl chloride)	CH ₂ :CHCH ₂ Cl	76.53	107-05-1	-136	45.7	0.938(20/4)	
- 1-Chloro-2-methyl-1-propene	(CH ₃) ₂ C:CHCl	90.55	513-37-1		68	0.92	
- 3-Chloro-2-methyl-1-propene	CH ₂ :C(CH ₃)CH ₂ Cl	90.55	563-47-3		71~73	0.9165~0.928(20/4)	
1,1-Dichloropropene	CH ₂ CH:CCl ₂	110.97	563-58-6	液体	77	1.18	
1,2-Dichloropropene	CH ₂ CCl:CHCl	110.97	563-54-4	液体	(E)74.2(732mmHg) (Z)92.5(742mmHg)	1.18	
- cis-1,3-Dichloropropene	ClCH ₂ CH:CHCl	110.97	10061-01-5	液体	112.3	1.224(20/4)	
- trans-1,3-Dichloropropene	ClCH ₂ CH:CHCl	110.97	10061-02-6	液体	104.3	1.217(20/4)	
- 2,3-Dichloropropene	ClCH ₂ CCl:CH ₂	110.97	78-88-6	液体	94	1.22	
3,3-Dichloropropene	Cl ₂ CHCH:CH ₂	110.97	563-57-5	液体	84.4		
1,2,3-Trichloropropene	ClCH:C(Cl)CH ₂ Cl	145.41	96-19-5		145	1.43	
Tetrachloropropene	CH ₃ CH:CH ₂ →Cl ₄	179.86	60320-18-5?				
Pentachloropropene	C ₃ HCl ₅	214.31	69102-77-8				
1,1,2,3,3-Pentachloropropene	Cl ₂ C:CHCCl ₃	214.31	1600-37-9				
1,1,3,3,3-Pentachloropropene	Cl ₂ C:CHCCl ₃	214.31	6262-54-0				
Dichloropropadiene	CH ₂ :C:CH ₂ →Cl ₂	108.95					
Trichloropropadiene	CCl ₂ :C:CHCl	143.4	20170-70-1				
Tetrachloropropadiene	CCl ₂ :C:CCl ₂	177.84	18608-30-5				
- Hexachlorocyclopentadiene	CCl ₂ CCl:CClCCl:CCl	272.77	77-47-4				
- 1-Bromobutane(n-Butyl bromide)	CH ₃ (CH ₂) ₃ Br	137.02	109-65-9			1.712(20/4)	
2-Bromobutane(sec-Butyl bromide)	CH ₃ CHBrCH ₂ CH ₃	137.02	78-76-2			1.278(20/4)	
# Tetrachlorobutene	C ₄ H ₄ Cl ₄	193.90					

表 1. 微量有機化合物の一覧表

No. 17

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
** Trichlorobutatriene	ClHC:C:CCl ₂	155.41					
** Tetrachlorobutatriene	Cl ₂ C:C:CCl ₂	189.86	19792-18-8				
- 1,2-Butadiene	CH ₃ CH:C:CH ₂	54.09	590-19-2	液体	18~19	0.650(/-6)	
- 1,3-Butadiene	CH ₂ CHCH:CH ₂	54.09	106-99-0		-5(713mmHg)		
Tetrachlorobutadiene	C ₂ H ₂ Cl ₄	191.89	58334-79-5				
1,1,2,3-Tetrachlorobutadiene	C ₂ H ₂ Cl ₄	191.89	921-09-5				
1,1,4,4-Tetrachlorobutadiene	C ₂ H ₂ Cl ₄	191.89	36038-53-6				
1,2,3,4-Tetrachlorobutadiene	C ₂ H ₂ Cl ₄	191.89	1637-31-6				
Pentachlorobutadiene	CH ₂ :CHCH:CH ₂ →:Cl ₂	226.32	55880-77-8				
cis-Pentachlorobutadiene	CH ₂ :CHCH:CH ₂ →:Cl ₂	226.32	21484-04-8				
trans-Pentachlorobutadiene	CH ₂ :CHCH:CH ₂ →:Cl ₂	226.32	21484-05-9				
Hexachloro-1,3-butadiene	Cl ₂ C:CClCCl:CCl ₂	260.76	87-68-3			1.683(20/4)	
** Chloromethylbutene	CH ₂ :C(CH ₃)CH ₂ CH ₂ →:Cl	104.58	68012-28-2				
** Bromomethylbutene	CH ₂ :C(CH ₃)CH ₂ CH ₂ →:Br	149.03					
** Hexachlorohexatriene	CH ₂ :CHCH:CHCH:CH ₂ →:Cl ₂	286.8					
** Heptachlorohexatriene	CH ₂ :CHCH:CHCH:CH ₂ →:Cl ₂	321.24					
Heptane	CH ₃ (CH ₂) ₅ CH ₃	100.20	142-82-5	-90	98.4	0.684(20/4)	0.005%(15°C)
- 2,4,4-Trimethyl-1-pentene	(CH ₃) ₂ CCH ₂ C(CH ₃):CH ₂	112.22	107-39-1				
2,4,4-Trimethyl-2-pentene	(CH ₃) ₂ CCH:CHC(CH ₃) ₂	112.22	107-40-4				
+ Cyclopentane	CH ₂ (CH ₂) ₃ CH ₂	70.14	287-92-3	-93.3	49~50	0.745~0.751(20/4)	不溶
芳香族炭化水素							
+ Dicyclopentadiene	C ₁₀ H ₁₂	132.21	77-73-6			0.981(20/4)	
- Cyclohexanone	C ₆ H ₁₀ O	98.14	108-94-1	-26	156~157	0.948(20/20)	溶解
# Cyclohexene	C ₆ H ₁₀	82.15	110-83-8	-103.7	83.3	0.811(20/4)	微溶
- Chlorocyclohexene	C ₆ H ₉ Cl	118.61	542-18-7	-43.9	143	1.004(20/4)	不溶
Limone	C ₁₀ H ₁₆	136.24	138-86-3				
# D-Limonene	C ₁₀ H ₁₆	136.24	5989-27-5	-96.9	178	0.8411(20/4)	不溶
DL-Limonene	C ₁₀ H ₁₆	136.24	7705-14-8	液体	178	0.844(20/4)	不溶
L-Limonene	C ₁₀ H ₁₆	136.24	5989-54-8				
Terpinolene	C ₁₀ H ₁₆	136.24	586-62-9		186~187	0.862(20/4)	不溶
Benzene	C ₆ H ₆	78.11	71-43-2	5.29~5.5	80.13	0.879(20/20)	不溶
** Chlorobenzene	C ₆ H ₅ Cl	112.56	108-90-7	-45	132	1.106~1.109(20/4)	不溶
- Bromobenzene	C ₆ H ₅ Br	157.01	108-86-1		156.2	1.4952(20/4)	0.045%(30°C)
+ Nitrobenzene	C ₆ H ₅ NO ₂	123.11	98-95-3	5.7	210.9	1.206(20/20)	不溶
- o-Chloronitrobenzene	ClC ₆ H ₄ NO ₂	157.56	88-73-3	32.33	245~246	1.305	不溶
- m-Chloronitrobenzene	ClC ₆ H ₄ NO ₂	157.56	121-73-3	46	236	1.534(20/4)	不溶
- p-Chloronitrobenzene	ClC ₆ H ₄ NO ₂	157.56	100-00-5	81~85	242	1.520	不溶
- 1-Chloro-2,4-dinitrobenzene	(NO ₂) ₂ C ₆ H ₃ Cl	202.55	97-00-7	50~54	315	1.687(17/)	不溶
(2,4-Dinitrochlorobenzene)							
- Chloro-3,4-dinitrobenzene	(NO ₂) ₂ C ₆ H ₃ Cl	202.55	610-40-2	36.3			
** o-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.01	95-50-1	-17	179.2	1.310(20/4)	
** m-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.01	541-73-1	-24.4	172(766mmHg)	1.288~1.291(20/4)	
** p-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.01	106-46-7	54	174.5	1.248(58/4)	不溶
- o-Dibromobenzene	C ₆ H ₃ Br ₂	235.91	583-53-9	6.7	225	1.956(20/)	
- m-Dibromobenzene	C ₆ H ₃ Br ₂	235.91	108-36-1	-6.9	220	1.952(20/)	

表 1. 微量有機化合物の一覧表

No. 18

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
- p-Dibromobenzene	C ₆ H ₄ Br ₂	235.91	106-37-6	89	219	2.268(0/)	
- o-Dinitrobenzene	C ₆ H ₄ (NO ₂) ₂	168.11	528-29-0	116~119	319(773mmHg)	1.565(17/)	0.01%
- m-Dinitrobenzene	C ₆ H ₄ (NO ₂) ₂	168.11	99-65-0	89~91	297	1.575(18/)	0.007%
- p-Dinitrobenzene	C ₆ H ₄ (NO ₂) ₂	168.11	100-25-4	171~175	299(777mmHg)	1.625(18/)	0.01%
- 2,3-Dichloronitrobenzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	3209-22-1	61~62	257~258	1.449(80/)	不溶
- 2,4-Dichloronitrobenzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	611-06-3	33	258.5	1.439(80/)	
- 2,5-Dichloronitrobenzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	89-61-2	52~56	267	1.669(22/)	
- 3,4-Dichloronitrobenzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	99-54-7	39~43	255~256	1.451(80/)	不溶
- 3,5-Dichloronitrobenzene	Cl ₂ C ₆ H ₃ NO ₂	192.00	618-62-2	62~65.4		1.428(80/)	不溶
** 1,2,3-Trichlorobenzene	C ₆ H ₃ Cl ₃	181.45	87-61-6	51~55	218~221		不溶
** 1,2,4-Trichlorobenzene	C ₆ H ₃ Cl ₃	181.45	120-82-1	17~18	212~213	1.465(20/20)	不溶
** 1,3,5-Trichlorobenzene	C ₆ H ₃ Cl ₃	181.45	108-70-3	63.4	208.4		不溶
- 1,2,4-Tribromobenzene	C ₆ H ₃ Br ₃	314.80	615-54-3	44~45	275~276		不溶
- 1,3,5-Tribromobenzene	C ₆ H ₃ Br ₃	314.80	626-39-1	119~123	271(765mmHg)		不溶
- 2,3,4-Trichloronitrobenzene	C ₆ H ₂ Cl ₃ NO ₂	226.45	17700-09-3	56			
- 2,4,5-Trichloronitrobenzene	Cl ₃ C ₆ H ₂ NO ₂	226.45	89-69-0	58			
- 2,4,6-Trichloronitrobenzene	Cl ₃ C ₆ H ₂ NO ₂	226.45	18708-70-8	72	254(761mmHg)		不溶
** 1,2,3,4-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.89	634-66-2	43~47.5	246		不溶
** 1,2,3,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.89	634-90-2	52~55	243~246	1.859(22/4)	不溶
** 1,2,4,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.89	95-94-3	140~141	275~277	1.834(17/4)	不溶
** Pentachlorobenzene	C ₆ HCl ₅	250.35	608-93-5	85~86			
- Pentabromobenzene	C ₆ HBr ₅	424.6	608-90-2	56~57	210(300mmHg)		
** Hexachlorobenzene	Cl ₆ C ₆	295.34	82-68-8	144~147	328		不溶
** Hexabromobenzene	Br ₆ H ₆	551.49	87-82-1	326	322.2	2.044(23/4)	不溶
** Toluene	C ₆ H ₅ CH ₃	92.13	108-88-3	-95	昇華		不溶
- o-Chlorotoluene	ClC ₆ H ₄ CH ₃	126.59	95-49-8	-35.1	110.6~110.8	0.868(20/20)	不溶
- m-Chlorotoluene	ClC ₆ H ₄ CH ₃	126.59	108-41-8	-47.8	159.3	1.088(20/4)	不溶
- p-Chlorotoluene	ClC ₆ H ₄ CH ₃	126.59	106-43-4	7.8	161.6	1.076(20/4)	不溶
- Benzyl chloride	C ₆ H ₅ CH ₂ Cl	126.59	100-44-7	-39	162.4	1.069~1.074(20/4)	不溶
- 2,3-Dichlorotoluene	CH ₃ C ₆ H ₃ Cl ₂	161.03	32768-54-0		179.3	1.103(20/20)	不溶
- 2,4-Dichlorotoluene	CH ₃ C ₆ H ₃ Cl ₂	161.03	95-73-8			1.270(20/4)	
- 2,5-Dichlorotoluene	CH ₃ C ₆ H ₃ Cl ₂	161.03	118-69-4			1.251(20/4)	
- 2,6-Dichlorotoluene	CH ₃ C ₆ H ₃ Cl ₂	161.03	19398-61-9				
- 3,4-Dichlorotoluene	CH ₃ C ₆ H ₃ Cl ₂	161.03	95-75-0			1.267(20/4)	
+ o-Nitrotoluene	C ₆ H ₄ (NO ₂)CH ₃	137.14	88-72-2	α-10.37, β-4.31	222.3	1.257(20/4)	不溶
+ m-Nitrotoluene	C ₆ H ₄ (NO ₂)CH ₃	137.14	99-08-1	15.6~16	231.87	1.164(20/4)	
+ p-Nitrotoluene	C ₆ H ₄ (NO ₂)CH ₃	137.14	99-99-0	50~54	238.34~238.5	1.160(20/4)	
- 2,4-Dinitrotoluene	C ₆ H ₃ (NO ₂) ₂ CH ₃	182.14	121-14-2	70.5~71		1.117(58/)	
+ 2,6-Dinitrotoluene	C ₆ H ₃ (NO ₂) ₂ CH ₃	182.14	606-20-2	66		1.518(15/)	0.027%(22°C)
- 3,4-Dinitrotoluene	C ₆ H ₃ (NO ₂) ₂ CH ₃	182.14	610-39-9	60		1.538(15/)	
+ o-Xylene	C ₆ H ₄ (CH ₃) ₂	106.16	95-47-6	-27.95~25	142~144	1.259(111/)	不溶
+ m-Xylene	C ₆ H ₄ (CH ₃) ₂	106.16	108-38-3	-47.45	139.3	0.881(20/4)	不溶
+ p-Xylene	C ₆ H ₄ (CH ₃) ₂	106.16	106-42-3	13.35	137~138.4	0.864(20/4)	不溶
** Ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	106.16	100-41-4	-95.01~94.4	136.15~136.25	0.861(20/4)	不溶
- 1,2,3-Trimethylbenzene (Hemellitene)	C ₆ H ₃ (CH ₃) ₃	120.20	526-73-8	<-15	175~176	0.866(20/20)	不溶

表 1. 微量有機化合物の一覧表

No. 19

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
- 1,2,4-Trimethylbenzene(Pseudocumene)	C ₉ H ₈ (CH ₃) ₃	120.20	95-63-6	-61.0	168.2	0.875(20/4)	不溶
- 1,3,5-Trimethylbenzene(Mesitylene)	C ₉ H ₆ (CH ₃) ₃	120.20	108-67-8	-52.7	164.6	0.863(20/4)	0.002%
+ n-Propylbenzene	C ₉ H ₈ CH ₂ CH ₂ CH ₃	120.19	103-65-1	-99.2	159.55	0.861(20/4)	不溶
* Isopropylbenzene(Cumene)	C ₉ H ₈ CH(CH ₃) ₂	120.19	98-82-8	-96.9	152.5	0.863(20/20)	不溶
* o-Cymene	CH ₃ C ₆ H ₄ CH(CH ₃) ₂	134.22	527-84-4	液体	175~176	0.874(20/)	不溶
m-Cymene	CH ₃ C ₆ H ₄ CH(CH ₃) ₂	134.22	535-77-3	液体	174.5	0.862(20/)	不溶
** 1-Isopropyl-4-methylbenzene(p-cymene)	CH ₃ C ₆ H ₄ CH(CH ₃) ₂	134.22	98-87-6	-73.25	176~177.1	0.857(20/4)	不溶
Chlorocumene	C ₉ H ₇ Cl	168.67	72403-13-5			1.02	
** Chloro-p-Cymene	(CH ₃) ₂ CHC ₆ H ₄ CH ₂ Cl	168.67	2051-18-5			1.26	
# Bromocumene	C ₉ H ₇ Br	213.12	2437-76-5				
Bromo-p-Cymene	(CH ₃) ₂ CHC ₆ H ₄ CH ₂ Br	213.13	65724-11-0				
** Dichloro-p-Cymene	(CH ₃) ₂ CHC ₆ H ₄ CHCl ₂	203.12	65724-12-1				
** Trichloro-p-Cymene	(CH ₃) ₂ CHC ₆ H ₄ CCl ₃	237.56					
# Bromochlorocumene	(CH ₃) ₂ CHC ₆ H ₄ CHBrCl	247.58					
- Diisopropylbenzene	C ₉ H ₈ [CH(CH ₃) ₂] ₂	162.27	25321-09-9		203	0.86	
- 1,3-Diisopropylbenzene	C ₉ H ₈ [CH(CH ₃) ₂] ₂	162.27	99-62-7			0.86	
- 1,4-Diisopropylbenzene	C ₉ H ₈ [CH(CH ₃) ₂] ₂	162.28	100-18-5				
+ Diphenylmethane	C ₆ H ₅ CH ₂ C ₆ H ₅	168.24	101-81-5	26~27	265.6	1.006(20/)	不溶
+ Styrene	C ₆ H ₅ CH=CH ₂	104.14	100-42-5	-31~-30.6	145.8	0.906(20/4)	微溶
- α-Methylstyrene	C ₆ H ₅ C(CH ₃):CH ₂	118.18	98-83-9	-24	54.5~55(14mmHg)	0.910(20/4)	
- β-Methylstyrene	C ₆ H ₅ CH:CHCH ₃	118.18	637-50-3		cis64.5(20mmHg) trans73.5(20mmHg)	cis0.9107(25/4) trans0.9019(25/4)	
- o-Methylstyrene	CH ₃ C ₆ H ₄ CH:CH ₂	118.18	611-15-4		55.4(12mmHg)	0.9111(20/4)	
- m-Methylstyrene	CH ₃ C ₆ H ₄ CH:CH ₂	118.18	100-80-1		61~62(18mmHg)	0.903(20/20)	
- p-Methylstyrene	CH ₃ C ₆ H ₄ CH:CH ₂	118.18	622-97-9		59~60(12mmHg)	0.900(16.4/4)	
- α-Chlorostyrene	C ₆ H ₅ CCl:CH ₂	138.18	618-34-8	-23	199		
- β-Chlorostyrene	C ₆ H ₅ CH:CHCl	138.18	622-25-3	液体	199		
- 2-Chlorostyrene	H ₂ C:CHC ₆ H ₄ Cl	138.60	2039-87-4		186.4		
- 3-Chlorostyrene	H ₂ C:CHC ₆ H ₄ Cl	138.60	2039-85-2		57.5~57.8(10mmHg)		
- 4-Chlorostyrene	H ₂ C:CHC ₆ H ₄ Cl	138.60	1073-67-2	-13	189.2	1.090(20/4)	
- α-Bromostyrene	C ₆ H ₅ CHBr:CH ₂	183.05	98-81-7	-44~-43	86~87(14mmHg)		
- β-Bromostyrene	C ₆ H ₅ CH:CHBr	183.05	103-64-0	cis-8 trans6.5	cis63.7~64.5(4mmHg) trans88(4mmHg)	1.422(20/)	0.009%
3-Bromostyrene	H ₂ C:CHC ₆ H ₄ Br	183.05	2039-86-3				
4-Bromostyrene	H ₂ C:CHC ₆ H ₄ Br	183.05	2039-82-9				
# Chloro-1-isopropenylbenzene	ClCH ₂ C ₆ H ₄ CH:CH ₂	152.62	30030-25-2			1.10	
p-Dichloroisopropenylbenzene	ClC ₆ H ₄ C(CH ₃):CH ₂	152.62	1712-70-5			1.07	
p-Dichloroisopropenylbenzene	C ₆ H ₅ Cl ₂	187.08	35325-11-2				
# Dichloro-1-isopropenylbenzene	Cl ₂ CHC ₆ H ₄ CH:CH ₂	187.08					
Calamenene	C ₁₅ H ₂₂	190.33	483-77-2				
(-)Calamenene	C ₁₅ H ₂₂	190.33	483-77-2				
(+)Calamenene	C ₁₅ H ₂₂	190.33	22339-23-7				
(±)Calamenene	C ₁₅ H ₂₂	190.33	29448-31-5				
cis-Calamenene	C ₁₅ H ₂₂	190.33	72937-55-4				
Chlorocalamenene	C ₁₅ H ₂₁ Cl	224.77					
# Bromocalamenene	C ₁₅ H ₂₁ Br	269.22					
- Naphthalene	C ₁₀ H ₈	128.18	91-20-3	80.05	218.05	1.168(22/4)	0.04%(25°C)

表 1. 微量有機化合物の一覧表

No. 20

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
- 1-Chloronaphthalene (α -)	C ₁₀ H ₇ Cl	162.62	90-13-1	-17~-2.5	259.3~262.7	1.194(20/4)	12.1%
- 2-Chloronaphthalene (β -)	C ₁₀ H ₇ Cl	162.62	91-58-7	56.7~61	264~266	1.266(16/4)	6.1%
- 1-Methylnaphthalene	C ₁₀ H ₇ (CH ₃)	142.20	90-12-0	-19	244.6~244.8	1.0163(25/4)	不溶
- 2-Methylnaphthalene	C ₁₀ H ₇ (CH ₃)	142.20	91-57-6	35.1	241.8~245	0.9905(25/4)	不溶
+ 1,2-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	573-98-8	-1.6	266.7	1.025(17/)	不溶
+ 1,3-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	575-41-7	-6	263	1.01	不溶
+ 1,4-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	571-58-4	<-20~-7.66	265~268	1.016(20/)	不溶
+ 1,5-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	571-61-9	81~83	265	1.006(15/)	不溶
- 1,6-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	575-43-9	液体	262~263		不溶
+ 1,8-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	569-41-5	57~65	270		不溶
+ 2,3-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	581-40-8	103~105	266~268		不溶
+ 2,6-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	581-42-0	108~112	261~262	1.142(0/)	不溶
- 2,7-Dimethylnaphthalene	C ₁₀ H ₆ (CH ₃) ₂	156.23	582-16-1	94~98	262		不溶
- 2-Isopropylnaphthalene	C ₁₂ H ₁₄	170.25	2027-17-0		268	0.98	
- 2,6-Diisopropylnaphthalene	C ₁₄ H ₂₀	212.33	38640-62-9			0.970(20/4)	
- Tetrahydronaphthalene	C ₁₀ H ₈	132.21	119-64-2			0.896(20/4)	
- cis-Decahydronaphthalene	C ₁₀ H ₁₈	138.25	493-01-6			0.870(20/4)	
- trans-Decahydronaphthalene	C ₁₀ H ₁₈	138.25	493-02-7				
* Chlorodimethylpropyldihydronaphthalene	C ₁₅ H ₂₀ Cl	235.78					
** Dichlorodimethylpropyldihydronaphthalene	C ₁₅ H ₁₈ Cl ₂	270.22					
# Chlorodimethylisopropylnaphthalene	C ₁₃ H ₁₆ (CH ₃) ₂ C ₃ H ₇	232.73					
# Dichlorodimethylisopropylnaphthalene	C ₁₃ H ₁₄ (CH ₃) ₂ C ₃ H ₇	267.19					
# Dichlorodimethylisopropylnaphthalene	C ₁₃ H ₁₄ (CH ₃) ₂ C ₃ H ₇	267.19					
- 1-Nitronaphthalene	C ₁₀ H ₇ NO ₂	173.17	86-57-7	55~61.5	304	1.223(62/)	0.005% (18°C)
- 2-Nitronaphthalene	C ₁₀ H ₇ NO ₂	173.17	581-89-5	79	182(14mmHg)		
- 1,5-Dinitronaphthalene	C ₁₀ H ₆ (NO ₂) ₂	218.17	605-71-0	217.5			0.006% (12°C)
- 1,8-Dinitronaphthalene	C ₁₀ H ₆ (NO ₂) ₂	218.17	602-38-0	171.5			0.003% (15°C)
# Pentylfuran	C ₄ H ₉ OC ₄ H ₉	138.21	64079-01-2			0.88	
2-Pentylfuran	C ₄ H ₉ O(CH ₂) ₄ CH ₃	138.21	3777-69-3			0.88	
3-Pentylfuran	C ₄ H ₉ O(CH ₂) ₄ CH ₃	138.21	6177-84-0				
イオウ化合物							
- Thiourea	H ₂ NCSNH ₂	76.12	62-56-6	176~178		1.405	
- Thioephane	C ₄ H ₄ S	84.14	110-02-1	-29.8~-38.3	84.4	1.066(20/20)	不溶
- Ethanethiol (Ethylmercaptan)	C ₂ H ₅ SH	62.14	75-08-1	-147	37	0.840(20/4)	難溶
- Methyl sulfide	(CH ₃) ₂ S	62.14	75-18-3		37	0.85	
- Dimethyl disulfide	(CH ₃) ₂ S ₂	94.20	624-92-0		110	1.06	
- Saccharin (o-Sulfobenzimide)	C ₇ H ₅ NO ₃ S	183.19	81-07-2	229	300(昇華)	0.828	
- N-Methylsaccharin	C ₈ H ₇ NO ₃ S	197.21	15448-99-4	131~134			
** Trichlorothiophene	C ₄ HCl ₃ S	187.48	26761-53-5				
2,3,4-Trichlorothiophene	C ₄ HCl ₃ S	187.48	17249-78-4				
2,3,5-Trichlorothiophene	C ₄ HCl ₃ S	187.48	17249-77-3				
** Tetrachlorothiophene	C ₄ Cl ₄ S	221.92	6012-97-1	28~30	75(2mmHg)	1.704	
- Bromotrachlorothiophene	C ₄ BrCl ₃ S	266.38					
- Tetrabromothiophene	C ₄ Br ₄ S	399.73	3958-03-0	115			
* Dichloro-2-formyl-thiophene	C ₅ H ₂ Cl ₂ SO	181.04					

表1. 微量有機化合物の一覧表

No.21

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
* Trichloro-2-formyl-thiophene	C ₅ HCl ₃ SO	214.47	66729-79-1				
* Chlorotrimethoxybenzene	ClC ₆ H ₃ (OCH ₃) ₃	202.64					
** Dichlorotrimethoxybenzene	Cl ₂ C ₆ H ₂ (OCH ₃) ₃	237.09					
** Trichlorotrimethoxybenzene	Cl ₃ C ₆ (OCH ₃) ₃	271.54					
** 1,1-Dichlorodimethylsulphone	Cl ₂ CHS(:O) ₂ CH ₃	163.02	37557-97-4				
** 1,1,3-Trichlorodimethylsulphone	Cl ₂ CHS(:O) ₂ CH ₂ Cl	197.46					
# 1,1,3,3-Tetrachloro-dimethylsulphone	Cl ₄ CHS(:O) ₂ CHCl ₂	231.93					
Diphenyl disulfide	C ₆ H ₅ SSC ₆ H ₅	218.34	882-33-7	58~62	310		不溶
窒素化合物							
Cyanogen chloride	ClCN	61.5	506-77-4	-6.9~-6	12.7~13.8	1.186(20/)	易溶
Cyanogen bromide	BrCN	105.92	506-68-3	49~53	61~62	2.015(20/4)	易溶
+ Acetonitrile	CH ₃ CN	41.05	75-05-8	-44.9	81.6	0.784(20/20)	無限
Chloroacetonitrile	ClCH ₂ CN	75.50	107-14-2		124~126(126mmHg)	1.193~1.200(20/4)	
Dichloroacetonitrile	Cl ₂ CHCN	109.94	3018-12-0		110~113	1.369(20/)	
Trichloroacetonitrile	Cl ₃ CN	144.39	545-06-2	-42	75.6~85.7	1.440(20/4)	
Bromoacetonitrile	BrCCN	157.38	83463-62-1		125~130	1.68(20/)	
Dibromoacetonitrile	Br ₂ CHCN	198.86	3252-43-5		169	2.30(20/)	
Bromoacetonitrile	BrCH ₂ CN	119.95	590-17-0		60~62(24mmHg)	1.722~1.80	
- Propionitrile	CH ₃ CH ₂ CN	55.08	107-12-0	-103.5~-91.9	97.1	0.784(20/4)	1%以上
2-Chloropropionitrile	CH ₃ CH(Cl)CN	89.52	1617-17-0		120~122	1.012	
3-Chloropropionitrile	ClCH ₂ CH ₂ CN	89.52	542-76-7	-51	176	1.148(20/4)	2.2%(25°C)
3-Bromopropionitrile	BrCH ₂ CH ₂ CN	133.98	2417-90-5		76~78(10mmHg)	1.615	
- Isobutyronitrile	(CH ₃) ₂ CHCN	69.11	78-82-0		108	0.770(20/4)	1%以上
- Acrylonitrile	CH ₂ =CHCN	53.06	107-13-1	-83	77.3	0.806~0.808(20/4)	0.001%以上
- Adiponitrile	NCCH ₂ (CH ₂) ₄ CN	108.14	111-69-3			0.964(20/4)	
- 2,2-Azobisisobutyronitrile	(CH ₃) ₂ C(CN)N:NC(CN)(CH ₃) ₂	164.21	78-67-1				
- Benzonitrile	C ₆ H ₅ CN	103.12	100-47-0	-13	191	1.006(20/4)	
- Phthalonitrile	C ₆ H ₄ (CN) ₂	128.13	91-15-6	138~142	150~152(10mmHg)		
- Isophthalonitrile	C ₆ H ₄ (CN) ₂	128.13	626-17-5	159~163			
- Chloropiridin(Trichloronitromethane)	CCl ₃ NO ₂	165.00	76-06-2	-64	112	1.6558(20/4)	可溶
- Bromodichloronitromethane	BrCl ₂ NO ₂	208.85	918-01-4		52(20mmHg)	2.073(25/)	0.16%
- Dibromochloronitromethane	Br ₂ ClNO ₂	253.31	1184-89-0		67~69(22mmHg)	2.398(25/)	
- Tribromonitromethane	Br ₃ NO ₂	297.7	464-10-8	10	89~90(20mmHg)		
- Bromochloronitromethane	CHBrClNO ₂	174.4	135531-25-8				
+ Pyridine	C ₅ H ₅ N	79.10	110-86-1	-42	115.5	0.978(25/)	無限
- 2-Chloropyridine	C ₅ H ₄ NC1	113.55	109-09-1	液体	171	1.212(20/4)	不溶
- 3-Chloropyridine	C ₅ H ₄ NC1	113.55	626-60-8	液体	148(744mmHg)		可溶
+ 2-Methylpyridine(α-Picoline)	C ₅ H ₇ NCH ₃	93.13	109-06-8	-66.6~-69.9	129	0.946(20/4)	溶解
+ 3-Methylpyridine(β-Picoline)	C ₅ H ₇ NCH ₃	93.13	108-99-6	-17.7	143.4~144	0.956(20/4)	無限
+ 4-Methylpyridine(γ-Picoline)	C ₅ H ₇ NCH ₃	93.13	108-89-4	4.3	143.1~145	0.955(20/4)	溶解
- 2-Aminopyridine	C ₅ H ₆ N(NH ₂)	94.12	504-29-0	57~61	204~210.6		易溶
- 3-Aminopyridine	C ₅ H ₆ N(NH ₂)	94.12	462-08-8	59~65	251~252		易溶
- 4-Aminopyridine	C ₅ H ₆ N(NH ₂)	94.12	504-24-5	157~163			易溶
- 2-Cyanopyridine	N:CHC(CN)CH:CHCH:CH	104.11	100-70-9	29	212		易溶
- 3-Cyanopyridine	N:CHC(CN)CH:CHCH:CH	104.11	100-54-9	47~52	240~245		可溶

表 1. 微量有機化合物の一覧表

No. 22

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
- 4-Cyanopyridine	N:CHC(CN)CH:CHCH:CH	104.11	100-48-1	77~83			可溶
- 2-Vinylpyridine	N:C(CH:CH ₂)CH:CHCH:CH	105.14	100-69-6			0.976(20/4)	
- 4-Vinylpyridine	N:C(CH:CH ₂)CH:CHCH:CH	105.14	100-43-6			0.987(20/4)	
- N,N-Dimethyl-p-nitrosoaniline	NO ₂ C ₆ H ₄ N(CH ₃) ₂	150.18	138-89-6	84~87			
+ o-Nitroanisole	NO ₂ C ₆ H ₄ OCH ₃	153.14	91-23-6	10	265	1.253(20/)	0.167%(30°C)
+ m-Nitroanisole	NO ₂ C ₆ H ₄ OCH ₃	153.14	555-03-3				
- p-Nitroanisole	NO ₂ C ₆ H ₄ OCH ₃	153.14	100-17-4	54	258~260	1.233(20/)	
- 2-Chloroanisole	ClC ₆ H ₄ OCH ₃	142.58	766-51-8			1.195(20/4)	
- 3-Chloroanisole	ClC ₆ H ₄ OCH ₃	142.58	2845-89-8			1.175(20/4)	
- 4-Chloroanisole	ClC ₆ H ₄ OCH ₃	142.58	623-12-1				
- 2,3-Dichloroanisole	Cl ₂ C ₆ H ₃ OCH ₃	177.03	1984-59-4				
- 2,6-Dichloroanisole	Cl ₂ C ₆ H ₃ OCH ₃	177.03	1984-85-2				
- 2,3,4-Trichloroanisole	Cl ₃ C ₆ H ₂ OCH ₃	211.47	54135-80-7	70			
- 2,3,6-Trichloroanisole	Cl ₃ C ₆ H ₂ OCH ₃	211.47	50375-10-5	45			
- 2,4,6-Trichloroanisole	Cl ₃ C ₆ H ₂ OCH ₃	211.47	87-40-1	60			
- ε-Caprolactam	C ₆ H ₁₁ NO	113.16	105-60-2	68~71	180(50mmHg)	1.02(75/4)	微溶
+ Quinoline	C ₈ H ₇ N	129.16	91-22-5	-15	237.7	1.090(20/20)	難溶(熱水に可溶)
+ Aniline	C ₆ H ₅ NH ₂	93.13	62-53-3	-5.98	184.5	1.023(20/20)	3.66%
+ o-Chloroaniline	ClC ₆ H ₄ NH ₂	127.57	95-51-2	-1.9~10.2	207.8	1.216(20/4)	0.38%
+ m-Chloroaniline	ClC ₆ H ₄ NH ₂	127.57	108-42-9	-10.2	230.5	1.221(20/4)	0.54%
+ p-Chloroaniline	ClC ₆ H ₄ NH ₂	127.57	106-47-8	69~72.5	232.3(昇華)		0.03%
- o-Bromoaniline	BrC ₆ H ₄ NH ₂	172.02	615-36-1	32	229	1.578(20/)	不溶
- m-Bromoaniline	BrC ₆ H ₄ NH ₂	172.02	591-19-5	18~18.8	251	1.584(20/4)	
- p-Bromoaniline	BrC ₆ H ₄ NH ₂	172.02	106-40-1	61~66	分解	1.799(18/)	
- 2,3-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	608-27-5	24	252		微溶
+ 2,4-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	554-00-7	60~64	242		難溶
- 2,5-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	95-82-9	48~51	251		
- 2,6-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	608-31-1	39			
+ 3,4-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	95-76-1	70~74	272		不溶
- 3,5-Dichloroaniline	Cl ₂ C ₆ H ₃ NH ₂	162.02	626-43-7	47~52	260		
+ 2,3,4-Trichloroaniline	Cl ₃ C ₆ H ₂ NH ₂	194.46	634-67-3	67.5	292(774mmHg)		微溶
- 2,4,5-Trichloroaniline	Cl ₃ C ₆ H ₂ NH ₂	194.46	636-30-6	92~98	270		微溶
- 2,4,6-Trichloroaniline	Cl ₃ C ₆ H ₂ NH ₂	194.46	634-93-5	75~80	262(746mmHg)		
+ N-Methylaniline	C ₆ H ₅ NHCH ₃	107.16	100-61-8	-57	195.7~204.7	0.988(20/4)	不溶
- 2-Chloro-4-methylaniline	ClC ₆ H ₄ (CH ₃)NH ₂	141.60	615-65-6				
- 2-Chloro-5-methylaniline	ClC ₆ H ₄ (CH ₃)NH ₂	141.60	95-81-8				
- 2-Chloro-6-methylaniline	ClC ₆ H ₄ (CH ₃)NH ₂	141.60	87-63-8				
- 3-Chloro-4-methylaniline	ClC ₆ H ₄ (CH ₃)NH ₂	141.60	95-74-9				
- 4-Chloro-2-methylaniline	ClC ₆ H ₄ (CH ₃)NH ₂	141.60	95-69-2				
- 5-Chloro-2-methylaniline	ClC ₆ H ₄ (CH ₃)NH ₂	141.60	95-79-4				
- 2,3-Dimethylaniline(2,3-Xylidine)	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.18	87-59-2	<-15	221~222	0.995(20/4)	0.02%
- 2,4-Dimethylaniline(2,4-Xylidine)	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.18	95-68-1	16~49	214~226	0.978(20/4)	0.03%
- 2,5-Dimethylaniline(2,5-Xylidine)	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.18	95-78-3	15.5	215(739mmHg)	0.977(20/4)	
- 2,6-Dimethylaniline(2,6-Xylidine)	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.18	87-62-7	液体	216	0.980(20/4)	
- 3,4-Dimethylaniline(3,4-Xylidine)	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.18	95-64-7	51	212~226	0.978(20/)	0.04%
+ 3,5-Dimethylaniline(3,5-Xylidine)	(CH ₃) ₂ C ₆ H ₃ NH ₂	121.18	108-69-0	<-20	220~221	0.972(20/20)	

表1. 微量有機化合物の一覧表

No.23

化合物名 (英語名)	化学式	分子量	Cas番号	融点	沸点	比重	水への溶解性
+ N,N-Dimethylaniline	$C_6H_5(NHCH_3)_2$	121.18	121-69-7	2.45	193.50	0.958(20/4)	
+ N-Ethylaniline	$C_6H_5NHC_2H_5$	121.18	103-69-5	-63.5~57	196.1~206	0.961(20/4)	
- N,N-Diethylaniline	$C_6H_5N(C_2H_5)_2$	149.24	91-66-7	-38.1~2.5	192.5~216.5	0.934(20/4)	不溶
- o-Nitroaniline	$C_6H_4(NO_2)NH_2$	138.13	88-74-4	70~74	165~168(25mmHg)	1.442(15/)	0.121%(25°C)
- m-Nitroaniline	$C_6H_4(NO_2)NH_2$	138.13	99-09-2	114	> 285	1.398(18/)	0.09%(25°C)
- p-Nitroaniline	$C_6H_4(NO_2)NH_2$	138.13	100-01-6	147~150		1.424	0.1136%
- 2-Chloro-4-nitroaniline	$ClC_6H_3(NO_2)NH_2$	172.57	121-87-9				
- 2-Chloro-5-nitroaniline	$ClC_6H_3(NO_2)NH_2$	172.57	6283-25-6	117~121			
- 4-Chloro-2-nitroaniline	$ClC_6H_3(NO_2)NH_2$	172.57	89-63-4	115~121			
- 4-Chloro-3-nitroaniline	$ClC_6H_3(NO_2)NH_2$	172.57	635-22-3	99~105			
- 5-Chloro-2-nitroaniline	$ClC_6H_3(NO_2)NH_2$	172.57	1635-61-6				
- 4-Ethoxylaniline(o-Phenetidine)	$C_6H_5OC_2H_4NH_2$	137.18	94-70-2	<-20	232.5	1.051(20/4)	0.0059%
- 2,4-Dinitroaniline	$C_6H_3(NO_2)_2NH_2$	183.12	97-02-9	177~188		1.615(14/)	不溶
- 2,6-Dinitroaniline	$C_6H_3(NO_2)_2NH_2$	183.12	606-22-4	137~140			
- 3,5-Dinitroaniline	$C_6H_3(NO_2)_2NH_2$	183.12	618-87-1	87~92			
- 2-Methyl-3-nitroaniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	603-83-8				
- 2-Methyl-4-nitroaniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	99-52-5	129~133			
- 2-Methyl-5-nitroaniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	99-55-8	104~108			
- 2-Methyl-6-nitroaniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	570-24-1	93~97			
- 4-Methyl-2-nitroaniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	89-62-3	113~118			
- 4-Methyl-3-nitroaniline	$CH_3C_6H_3(NO_2)NH_2$	152.15	119-32-4	76~81			
- Methylaniline	CH_3NH_2	31.06	74-89-5	-93~-92.5	-6.5~-6.3	0.699(-11/)	1153.9%
- Dimethylaniline	$(CH_3)_2NH$	45.09	124-40-3	-96	-6.9~7	0.680(0/)	易溶
- Trimethylaniline	$(CH_3)_3N$	59.11	75-50-3	-124~-117	2.87~3	0.662(-5/)	易溶
- Ethylaniline	$CH_3CH_2NH_2$	45.08	75-04-7	-83.3	16.6	0.689(15/)	無限
- Diethylaniline	$(C_2H_5)_2NH$	73.14	109-89-7	-48		0.705(20/4)	易溶
- Triethylaniline	$(C_2H_5)_3N$	101.19	121-44-8	-114.8	89.5	0.725(20/4)	無限
- Propylaniline	$CH_3CH_2CH_2NH_2$	59.11	107-10-8	-83.0	47.8	0.718(20/4)	無限
- Isopropylaniline	$(CH_3)_2CHNH_2$	59.11	75-31-0	-101.2	33	0.691(20/4)	無限
- Di-n-propylaniline(1,1-Iminodipropene)	$(C_3H_7)_2NH$	101.19	142-84-7	-63.0	109.2	0.739(20/4)	
- Diisopropylaniline(2,2-Iminodipropene)	$[(CH_3)_2CH]_2NH$	101.19	108-18-9			0.716(20/4)	
- n-Butylaniline	$CH_3(CH_2)_3NH_2$	73.14	109-73-9	-50.5	77.8	0.740(20/4)	無限
- Di-n-butylaniline	$(C_4H_9)_2NH$	129.25	111-92-2	-60	159	0.761(20/4)	0.6%
- Tri-n-butylaniline	$(C_4H_9)_3N$	185.36	102-82-9		216	0.780(20/4)	0.00021%
- n-Octylaniline	$CH_3(CH_2)_7NH_2$	129.25	111-86-4	液体	180	0.781(20/4)	
- Trioctylaniline	$[CH_3(CH_2)_7]_3N$	353.68	1116-76-3			0.811(20/4)	
+ Cyclohexylaniline	$C_6H_{11}NH_2$	99.18	108-91-8	液体	134.5	0.866(20/4)	微溶
- Allylaniline	$CH_2=CHCH_2NH_2$	57.10	107-11-9	液体	53.2	0.763(20/4)	無限
- Diallylaniline	$(CH_2=CHCH_2)_2NH$	97.16	124-02-7			0.789(20/4)	
- Triallylaniline	$(CH_2=CHCH_2)_3N$	137.23	102-70-5			0.800(20/4)	
- Ethylenedianiline	$H_2NCH_2CH_2NH_2$	60.10	107-15-3	8.5	117	0.895(20/4)	易溶
- 1,2-Propanedianiline	$CH_3CH(NH_2)CH_2NH_2$	74.13	78-90-0		119~200	0.863(20/4)	可溶
- 1,3-Propanedianiline	$H_2NCH_2CH_2CH_2NH_2$	74.13	109-76-2	-23.5	135~136(733mmHg)	0.887(20/4)	易溶
- Hexamethylenedianiline	$NH_2(CH_2)_6NH_2$	116.21	124-09-4	42	205(昇華)		無限
- Ethanolamine(2-Aminoethanol)	$H_2NCH_2CH_2OH$	61.09	141-43-5	油	171	1.017(20/4)	
- Diethanolamine(2,2-Iminodiethanol)	$NH(CH_2CH_2OH)_2$	105.14	111-42-2	28	268	1.097(20/)	

表1. 微量有機化合物の一覧表

No. 24

化合物名 (英語名)	化学式	分子重	Cas番号	融点	沸点	比重	水への溶解性
- Triethanolamine	$N(CH_2CH_2OH)_3$	149.19	102-71-6	20~21.2	277(150mmHg)	1.125(20/4)	無限
- 3-Propanolamine(3-Amino-1-propanol)	$NH_2CH_2CH_2CH_2OH$	75.11	156-87-6			0.990(20/4)	
- Isopropanolamine	$CH_3CH(OH)CH_2NH_2$	75.11	78-96-6				
+ Melanine	$C_3N_2(CH_2)_3$	126.12	108-78-1	(250~354)	昇華	1.573(14/)	0.029%(15°C)
+ Hexamethylenimine	$CH_2(CH_2)_6NH$	99.18	111-49-9	-37	138	0.879(20/4)	可溶
+ Acrylamide	$CH_2=CHCONH_2$	71.08	79-06-1	82~86	125(25mmHg)	1.122(30/4)	215.5%(30°C)
+ Diphenylamine	$(C_6H_5)_2NH$	169.23	122-39-4	53~55	302	1.159	0.003%(0°C)
+ o-Toluidine	$CH_3C_6H_4NH_2$	107.16	95-53-4	α -24.4, β -16.25	199.7	1.000(20/4)	1.5%(25°C)
+ m-Toluidine	$CH_3C_6H_4NH_2$	107.16	108-44-1	-31.5	203.3	0.990(20/4)	微溶
+ p-Toluidine	$CH_3C_6H_4NH_2$	107.16	106-49-0	43~45	200.3	0.970(40/)	0.713%(24°C)
- o-Phenylenediamine	$C_6H_4(NH_2)_2$	108.14	95-54-5	100~104	252~257	1.269(-78/)	4.1%
- m-Phenylenediamine	$C_6H_4(NH_2)_2$	108.14	108-45-2	62~65	285.5~287	1.139(15/15)	35.1%
- p-Phenylenediamine	$C_6H_4(NH_2)_2$	108.14	106-50-3	140~145.5	267		3.8~4.72%(25°C)
- Toluene-2,4-diamine	$CH_3C_6H_3(NH_2)_2$	122.17	95-80-7	95~101	292		3.5%
- Toluene-2,6-diamine	$CH_3C_6H_3(NH_2)_2$	122.17	823-40-5	100~106			5.2%
- Toluene-3,4-diamine	$CH_3C_6H_3(NH_2)_2$	122.17	496-72-0	86~99.5	285(昇華)		2.6%
+ o-Toluenesulfonamide	$CH_3C_6H_4SO_2NH_2$	171.22	88-19-7	152~158			0.16%(25°C)
+ p-Toluenesulfonamide	$CH_3C_6H_4SO_2NH_2$	171.22	70-55-3	134~139			0.32%(25°C)
+ o-Anisidine	$CH_3OC_6H_4NH_2$	123.7	90-04-0	5~6.22	225	1.096(20/4)	3.4%
+ m-Anisidine	$CH_3OC_6H_4NH_2$	123.7	536-90-3	-11	251	1.107(20/4)	0.2261%
+ p-Anisidine	$CH_3OC_6H_4NH_2$	123.7	104-94-9	57~60	243~246	1.061(67/)	2.39%
- 3,3-Dimethoxybenzidine	$CH_3OC_6H_3(NH_2)(NH_2)OCH_3$	244.29	119-90-4	135~139			
- α -Naphthylamine(1-Aminonaphthalene)	$C_{10}H_7NH_2$	143.19	134-32-7	49.2~50	299.4	1.108(50/)	0.167%
- β -Naphthylamine(2-Aminonaphthalene)	$C_{10}H_7NH_2$	143.19	91-59-8	110.1	306.1	1.031(142/)	0.0006%
- N-henyl-1-naphthylamine	$C_6H_5NHC_{10}H_7$	219.29	90-30-2				
- N-henyl-2-naphthylamine	$C_6H_5NHC_{10}H_7$	219.29	135-88-6				
- N-Nitrosodimethylamine	$(CH_3)_2NNO$	74.08	62-75-9				
- N-Nitrosodiethylamine	$(C_2H_5)_2NNO$	102.14	55-18-5				
+ N-Nitrosodiphenylamine	$C_6H_5N(NO)C_6H_5$	198.22	86-30-6	66.5~67.6			易溶
- 4-Nitrosodiphenylamine	$C_6H_5NHC_6H_4NO$	198.22	156-10-5	145	151~153	1.010(20/4)	溶解
					175~177	0.943(20/4)	0.0000036%

注1) 左端の# : 文献1に記載の有機化合物 左端の* : 文献2に記載の有機化合物

左端の+ : 文献3に記載してある有機化合物の内、公共水域で検出された物質 左端の- : 文献3に記載してある有機化合物の内、公共水域で不検出の物質

注2) 融点 : 単位は°Cである。

注3) 沸点 : 1気圧 (760mmHg) で測定し、単位は°Cである。1気圧以外で測定の場合には、()内にmmHgで表示してある。

注4) 比重 : ()内は左側の温度 (°C) において右側の温度 (°C) の水に対する比重測定条件である。()の無は室温 (15~20°C) における比重測定条件である。

注5) 水への溶解性 : ()内は溶解度の測定温度 (°C) である。()の無は室温 (15~20°C) における溶解度である。

この資料に記載された物質は表1の左端に#で印した。同様に文献2)は文献数179を参考にして書かれた総説であり、総説に記載された物質は*で印し、文献3)の調査物質数は732であり、この調査物質の内、公共水域で検出された物質は+で印し、不検出である物質は-で印した。無印は主に文献1)~4)の同族体・異性体、及び文献5)~10)等で記載された物質である。

文献1), 2)の多くの物質、文献4), 5), 9), 10)の一部の物質は現在汎用的に使用されているWiley, NBSの質量スペクトルライブラリーに未登録、または登録されていても不正確であるため、これらライブラリーは役に立たない場合が多くある。

なお、これら一覧表の内、アミン等は水道原水のみから検出されるが、水道水中から検出されない。しかし、その酸化物質が水道水から検出される。それら酸化物質の一部は未記載である。

3. まとめ

水道水及び水道原水中に存在、または可能性のある微量有機化合物の一覧表を作成した。欠落している物質が沢山あるので、皆様の批判、助言等により、改善したい。また香料、多環芳香族、有機金属化合物、ダイオキシン及び関連物質、有機リン酸トリエステル、フタル酸エステル、アジピン酸エステル、農薬等の化学物質とそれぞれの酸化物質を含めた水道水専用の質量スペクトルライブラリーが制作されることを強く熱望する。

これにより、ガスクロマトグラム上の未知ピークが解明され、水中における濃度レベルの把握が可能になる。これが結局、水道水の安全性確保・確認に寄与すると確信している。

謝 辞

今回、文献を提供してくださった摂南大学宮田秀明先生に深く感謝いたします。

要 約

著者らはパルプ工場排水、環境水中及び著者ら未発表の有機物の一覧表を基に、水道水及び水道原水中の微量有機化合物の一覧表を作成した。

但し、一覧表には中沸点及び高沸点である香料、多環芳香族、有機金属化合物、ダイオキシン及び関連物質、有機リン酸トリエステル、フタル酸エステル、アジピン酸エステル、農薬等の化学物質等は未記載である。

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