



Calculation of Volatile Compound Concentrations in Standard Solutions

Calculator of volatile compound concentrations in standard solutions prepared in the accordance of OIV methods, in $\mu\text{g/g}$ and $\text{g}/100 \text{ L AA}$

[GUIDE](#)[WES PARAMETERS](#)[MASSES \(A,B,C\)](#)[MASSES \(0,0.1,0.5,1,2\)](#)[MASSES \(D,E,QC,BT\)](#)[PEAK AREAS I](#)

Preparation of 40 % v/v Water Ethanol Solution (WES)

Measure 400 mL of absolute ethanol and pour it into a 1-liter volumetric flask. Bring the solution volume up to the 1-liter mark by adding distilled water and mix thoroughly.

Accurately determine the volumetric ethanol content in the WES (ABV_{WES} , %) and WES density using standard methods.

Enter the value of WES strength, in vol.% (from 10 to 100)

ABV_{WES} , vol.%:

Enter the value of WES density at a temperature of 20 °C, in $\text{kg/m}^3 = \text{g/l}$ (from 772 to 1000)

Density of WES, kg/m^3 :

[To button "Submit values" ->](#)

[Back to Main Menu ->](#)

Preparation of Standard Solution A

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette reagents into the flask one by one and weigh each reagent. Make up to volume with WES, mix thoroughly and weight it.

Determine the final mass of the flask with all reagents and WES added in the solution.

Enter the values:

Mass of empty flask for solution A, mg:

Mass of WES portion 1 added in solution A, m^{WES1}_A , mg:

Table SS-A. Purity P^i_i and mass values of the reagents m^i_A added in solution A

i	Reagent i	Purity P^i_i , %	Mass m^i_A , mg
1	acetaldehyde ▼	99.5	2000
2	ethyl acetate ▼	99.5	2000
3	acetal ▼	99.5	2000
4	methanol ▼	99.5	2000
5	2-butanol ▼	99.5	2000
6	n-propanol ▼	99.5	1990
7	2-methyl-1-propanol ▼	99.5	1980
8	n-butanol ▼	99.5	1960
9	2-methyl-1-butanol ▼	99.5	1950
10	3-methyl-1-butanol ▼	99.5	1950

Mass of WES portion 2 added in solution A, m^{WES2}_A , mg:

Final mass of flask with all compounds and WES added in solution A, mg:

Preparation of Standard Solution B

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette IS reagent into the flask and weigh it. Make up to volume with WES, mix thoroughly and weight it. Determine the final mass of the flask with IS reagent and WES added in the solution.

Enter the values:

Mass of empty flask for solution B, mg:

Mass of WES portion 1 added in solution B, m^{WES1}_B , mg:

Table SS-B. Purity P^{IS}_{IS} and mass value of IS m^{IS}_B added in solution B

Reagent IS name	Purity P^{IS}_{IS} , %	Mass m^{IS}_B , mg
4-methyl-1-pentanol ▼	99	2000

Mass of WES portion 2 added in solution B, m^{WES2}_B , mg:

Final mass of flask with all compounds and WES added in solution B, mg:

Preparation of Standard Solution C

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of solution A into the flask and 1 mL of solution B and weigh each compound. Make up to volume with WES and weight it.

Determine the final mass of the flask with all compounds and WES added in the solution.

Enter the values:

Mass of empty flask for solution C, mg:

Mass of WES portion 1 added in solution C, m^{WES1}_C , mg:

Table SS-C. Mass values m^A_C and m^B_C of the stock solutions A and B added in solution C

Mass m^A_C , mg	Mass m^B_C , mg
1000	1000

Mass of WES portion 2 added in solution C, m^{WES2}_C , mg:

Final mass of flask with all compounds and WES added in solution C, mg:

To button "Submit values" ->

[Back to Main Menu ->](#)

Preparation of Standard Solution 0

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of solution A into the flask and 1 mL of solution B and weigh each compound. Make up to volume with WES and weight it.

Determine the final mass of the flask with all compounds and WES added in the solution.

Enter the values:

Mass of empty flask for solution 0, mg:

Mass of WES portion 1 added in solution 0, m^{WES1}_0 , mg:

Table SS-0. Mass values m^A_0 and m^B_0 of the stock solutions A and B added in solution 0

Mass m^A_0 , mg	Mass m^B_0 , mg
0	1000

Mass of WES portion 2 added in solution 0, m^{WES2}_0 , mg:

Final mass of flask with all compounds and WES added in solution 0, mg:

Preparation of Standard Solution 0.1

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of solution A into the flask and 1 mL of solution B and weigh each compound. Make up to volume with WES and weight it.

Determine the final mass of the flask with all compounds and WES added in the solution.

Enter the values:

Mass of empty flask for solution 0.1, mg:

Mass of WES portion 1 added in solution 0.1, $m^{WES1}_{0.1}$, mg:

Table SS-0.1. Mass values $m^A_{0.1}$ and $m^B_{0.1}$ of the stock solutions A and B added in solution 0.1

Mass $m^A_{0.1}$, mg	Mass $m^B_{0.1}$, mg
100	1000

Mass of WES portion 2 added in solution 0.1, $m^{WES2}_{0.1}$, mg:

Final mass of flask with all compounds and WES added in solution 0.1, mg:

Preparation of Standard Solution 0.5

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of solution A into the flask and 1 mL of solution B and weigh each compound. Make up to volume with WES and weight it.

Determine the final mass of the flask with all compounds and WES added in the solution.

Enter the values:

Mass of empty flask for solution 0.5, mg:

Mass of WES portion 1 added in solution 0.5, $m^{WES1}_{0.5}$, mg:

Table SS-0.5. Mass values $m^A_{0.5}$ and $m^B_{0.5}$ of the stock solutions A and B added in solution 0.5

Mass $m^A_{0.5}$, mg	Mass $m^B_{0.5}$, mg
500	1000

Mass of WES portion 2 added in solution 0.5, $m^{WES2}_{0.5}$, mg:

Final mass of flask with all compounds and WES added in solution 0.5, mg:

Preparation of Standard Solution 1.0

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of solution A into the flask and 1 mL of solution B and weigh each compound. Make up to volume with WES and weight it.

Determine the final mass of the flask with all compounds and WES added in the solution.

Enter the values:

Mass of empty flask for solution 1.0, mg:

Mass of WES portion 1 added in solution 1.0, $m^{WES1}_{1.0}$, mg:

Table SS-1.0. Mass values $m^A_{1.0}$ and $m^B_{1.0}$ of the stock solutions A and B added in solution 1.0

Mass $m^A_{1.0}$, mg	Mass $m^B_{1.0}$, mg
1000	1000

Mass of WES portion 2 added in solution 1.0, $m^{WES2}_{1.0}$, mg:

Final mass of flask with all compounds and WES added in solution 1.0, mg:

Preparation of Standard Solution 2.0

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of solution A into the flask and 1 mL of solution B and weigh each compound. Make up to volume with WES and weight it.

Determine the final mass of the flask with all compounds and WES added in the solution.

Enter the values:

Mass of empty flask for solution 2.0, mg:

Mass of WES portion 1 added in solution 2.0, $m^{WES1}_{2.0}$, mg:

Table SS-2.0. Mass values $m^A_{2.0}$ and $m^B_{2.0}$ of the stock solutions A and B added in solution 2.0

Mass $m^A_{2.0}$, mg	Mass $m^B_{2.0}$, mg

Mass of WES portion 2 added in solution 2.0, $m^{WES2}_{2.0}$, mg:

Final mass of flask with all compounds and WES added in solution 2.0, mg:

[To button "Submit values" ->](#)

[Back to Main Menu ->](#)

Preparation of Standard Solution D

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of stock SS into the flask and weigh it. Make up to volume with WES and weight the second portion of WES.

Determine the final mass of the flask.

Enter the values:

Mass of empty flask for solution D, mg:

Mass of WES portion 1 added in solution D, m^{WES1}_D , mg:

Mass of SS-A added in solution D, m^A_D , mg:

Mass of WES portion 2 added in solution D, m^{WES2}_D , mg:

Final mass of flask with all compounds and WES added in solution D, mg:

Preparation of Standard Solution E

Weight the empty 100 mL volumetric flask. Measure approximately 60.0 mL of the WES, pour it into the flask and weight it.

Pipette the required amount of stock SS into the flask and weigh it. Make up to volume with WES and weight the second portion of WES.

Determine the final mass of the flask.

Enter the values:

Mass of empty flask for solution E, mg:

Mass of WES portion 1 added in solution E, m^{WES1}_E , mg:

Mass of SS-B added in solution E, m^B_E , mg:

Mass of WES portion 2 added in solution E, m^{WES2}_E , mg:

Final mass of flask with all compounds and WES added in solution E, mg:

Preparation of QC Solution

Weight the empty vessel (flask). Pipette 9 mL of solution D into the vessel and 1 mL of solution E and weigh each compound.

Thoroughly mix the contents of the vessel and determine the final mass of the flask.

Enter the values:

Mass of empty flask for solution QC, mg:

Mass of SS-D added in solution QC, m^D_{QC} , mg:

Mass of SS-E added in solution QC, m^E_{QC} , mg:

Final mass of flask with all compounds and WES added in solution QC, mg:

Preparation of BT Solution

Weight the empty vessel (flask). Pipette 9 mL of the WES into the vessel and 1 mL of solution E and weigh each compound.

Thoroughly mix the contents of the vessel and determine the final mass of the flask.

Enter the values:

Mass of empty flask for solution BT, mg:

Mass of WES portion added in solution BT, m^{WES}_{BT} , mg:

Mass of SS-E added in solution BT, m^E_{BT} , mg:

Final mass of flask with all compounds and WES added in solution BT, mg:

[To button "Submit values" ->](#)

[Back to Main Menu ->](#)

Data from chromatograms of solutions C for the estimation RRF and BT for blank test

Acquire 2-3 chromatograms of standard solutions C and BT. Measure peak areas for volatile compounds and ethanol and record the peak area values.

Table SS-C. Peak area values of compounds in calibration solution C

№	Compound	Pick area, units of area		
		1	2	3
1	acetaldehyde	0.012683464	0.012793685	0.012676084
2	ethyl acetate	0.020781086	0.020847225	0.020493309
3	acetal	0.02488721	0.025013307	0.024433204
4	methanol	0.015101409	0.01511946	0.014977001
5	2-butanol	0.028740452	0.029012715	0.028584787
6	n-propanol	0.027240509	0.027413972	0.027011264
7	2-methyl-1-propanol	0.031632479	0.031794037	0.031370909
8	n-butanol	0.03078556	0.031005659	0.03055382
9	2-methyl-1-butanol	0.034731363	0.03494925	0.034562455
10	3-methyl-1-butanol	0.032998299	0.033263599	0.032806384

11	<u>ethanol</u>	28.80839275	29.01551547	28.60029409
12	<u>4-methyl-1-pentanol</u>	0.034098982	0.03431334	0.033758576

Table SS-BT. Peak area values of compounds in blank test solution

№	Compound	Pick area, units of area		
		1	2	3
1	acetaldehyde	0.00012		
2	ethyl acetate	0.00027		
3	acetal	0.00019		
4	methanol	0.00031		
5	2-butanol	0		
6	n-propanol	0		
7	2-methyl-1-propanol	0		
8	n-butanol	0		
9	2-methyl-1-butanol	0		
10	3-methyl-1-butanol	0		
11	<u>ethanol</u>	28.80839		
12	<u>4-methyl-1-pentanol</u>	0.034092		

To button "Submit values" ->

[Back to Main Menu ->](#)

Concentrations of volatile compounds calculated using the TIS and EIS methods

Table SS-A. Concentrations of compounds in standard solution A

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	19935.58	5896.25	5896.20

2	ethyl acetate	19936.23	5896.44	5896.38
3	acetal	19935.26	5896.15	5896.12
4	methanol	19937.62	5896.85	5896.75
5	2-butanol	19933.89	5895.75	5895.75
6	n-propanol	19834.22	5866.27	5866.27
7	2-methyl-1-propanol	19734.55	5836.79	5836.79
8	n-butanol	19535.21	5777.83	5777.83
9	2-methyl-1-butanol	19435.54	5748.35	5748.35
10	3-methyl-1-butanol	19435.54	5748.35	5748.35
11	ethanol	266857.05	78927.00	78927.00
12	4-methyl-1-pentanol	0.00	0.00	0.00

[Download Data of Table SS-A ->](#)

Table SS-B. Concentrations of compounds in standard solution B

Nº	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	2.07	0.50	0.45
2	ethyl acetate	2.87	0.69	0.63
3	acetal	1.68	0.41	0.37
4	methanol	4.56	1.10	1.00
5	2-butanol	0.00	0.00	0.00
6	n-propanol	0.00	0.00	0.00
7	2-methyl-1-propanol	0.00	0.00	0.00
8	n-butanol	0.00	0.00	0.00
9	2-methyl-1-butanol	0.00	0.00	0.00
10	3-methyl-1-butanol	0.00	0.00	0.00
11	ethanol	326344.16	78927.00	78927.00
12	4-methyl-1-pentanol	19800.00	4788.67	4788.67

[Download Data of Table SS-B ->](#)

Table SS-C. Concentrations of compounds in standard solution C

Nº	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	201.43	47.85	47.80
2	ethyl acetate	202.24	48.04	47.97
3	acetal	201.03	47.75	47.71

4	methanol	203.95	48.44	48.34
5	2-butanol	199.34	47.35	47.35
6	n-propanol	198.34	47.11	47.11
7	2-methyl-1-propanol	197.35	46.88	46.88
8	n-butanol	195.35	46.40	46.40
9	2-methyl-1-butanol	194.36	46.17	46.17
10	3-methyl-1-butanol	194.36	46.17	46.17
11	ethanol	332276.17	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	47.03	47.03

[Download Data of Table SS-C ->](#)

Table SS-0. Concentrations of compounds in standard solution 0

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	2.11	0.50	0.45
2	ethyl acetate	2.93	0.69	0.63
3	acetal	1.71	0.41	0.37
4	methanol	4.65	1.10	1.00
5	2-butanol	0.00	0.00	0.00
6	n-propanol	0.00	0.00	0.00
7	2-methyl-1-propanol	0.00	0.00	0.00
8	n-butanol	0.00	0.00	0.00
9	2-methyl-1-butanol	0.00	0.00	0.00
10	3-methyl-1-butanol	0.00	0.00	0.00
11	ethanol	332937.64	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	46.94	46.94

Table SS-0.1. Concentrations of compounds in standard solution 0.1

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	22.04	5.23	5.18
2	ethyl acetate	22.86	5.42	5.35
3	acetal	21.64	5.13	5.09
4	methanol	24.58	5.83	5.72
5	2-butanol	19.93	4.73	4.73
6	n-propanol	19.83	4.70	4.70

7	2-methyl-1-propanol	19.73	4.68	4.68
8	n-butanol	19.54	4.63	4.63
9	2-methyl-1-butanol	19.44	4.61	4.61
10	3-methyl-1-butanol	19.44	4.61	4.61
11	ethanol	332871.49	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	46.95	46.95

Table SS-0.5. Concentrations of compounds in standard solution 0.5

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	101.77	24.15	24.10
2	ethyl acetate	102.58	24.34	24.28
3	acetal	101.37	24.06	24.02
4	methanol	104.30	24.75	24.64
5	2-butanol	99.67	23.65	23.65
6	n-propanol	99.17	23.53	23.53
7	2-methyl-1-propanol	98.67	23.41	23.41
8	n-butanol	97.68	23.18	23.18
9	2-methyl-1-butanol	97.18	23.06	23.06
10	3-methyl-1-butanol	97.18	23.06	23.06
11	ethanol	332606.90	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	46.99	46.99

Table SS-1.0. Concentrations of compounds in standard solution 1.0

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	201.43	47.85	47.80
2	ethyl acetate	202.24	48.04	47.97
3	acetal	201.03	47.75	47.71
4	methanol	203.95	48.44	48.34
5	2-butanol	199.34	47.35	47.35
6	n-propanol	198.34	47.11	47.11
7	2-methyl-1-propanol	197.35	46.88	46.88
8	n-butanol	195.35	46.40	46.40
9	2-methyl-1-butanol	194.36	46.17	46.17
10	3-methyl-1-butanol	194.36	46.17	46.17

11	ethanol	332276.17	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	47.03	47.03

Table SS-2.0. Concentrations of compounds in standard solution 2.0

Nº	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	400.74	95.38	95.33
2	ethyl acetate	401.54	95.57	95.51
3	acetal	400.35	95.29	95.25
4	methanol	403.24	95.97	95.87
5	2-butanol	398.68	94.89	94.89
6	n-propanol	396.68	94.41	94.41
7	2-methyl-1-propanol	394.69	93.94	93.94
8	n-butanol	390.70	92.99	92.99
9	2-methyl-1-butanol	388.71	92.52	92.52
10	3-methyl-1-butanol	388.71	92.52	92.52
11	ethanol	331614.70	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	47.13	47.13

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Table SS-D. Concentrations of compounds in standard solution D

Nº	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	201.43	47.84	47.79
2	ethyl acetate	202.24	48.03	47.96
3	acetal	201.03	47.74	47.70
4	methanol	203.95	48.43	48.33
5	2-butanol	199.34	47.34	47.34
6	n-propanol	198.34	47.10	47.10
7	2-methyl-1-propanol	197.35	46.87	46.87
8	n-butanol	195.35	46.39	46.39
9	2-methyl-1-butanol	194.36	46.16	46.16
10	3-methyl-1-butanol	194.36	46.16	46.16
11	ethanol	332342.77	78927.00	78927.00
12	4-methyl-1-pentanol	0.00	0.00	0.00

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Table SS-E. Concentrations of compounds in standard solution E

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	2.11	0.50	0.45
2	ethyl acetate	2.92	0.69	0.63
3	acetal	1.71	0.41	0.37
4	methanol	4.65	1.10	1.00
5	2-butanol	0.00	0.00	0.00
6	n-propanol	0.00	0.00	0.00
7	2-methyl-1-propanol	0.00	0.00	0.00
8	n-butanol	0.00	0.00	0.00
9	2-methyl-1-butanol	0.00	0.00	0.00
10	3-methyl-1-butanol	0.00	0.00	0.00
11	ethanol	332338.23	78927.00	78927.00
12	4-methyl-1-pentanol	1980.00	470.23	470.23

[Download Data of Table SS-E ->](#)
Table SS-QC. Concentrations of compounds in standard solution QC

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	181.49	43.10	43.06
2	ethyl acetate	182.30	43.29	43.23
3	acetal	181.10	43.01	42.97
4	methanol	184.02	43.70	43.60
5	2-butanol	179.40	42.61	42.61
6	n-propanol	178.51	42.39	42.39
7	2-methyl-1-propanol	177.61	42.18	42.18
8	n-butanol	175.82	41.75	41.75
9	2-methyl-1-butanol	174.92	41.54	41.54
10	3-methyl-1-butanol	174.92	41.54	41.54
11	ethanol	332342.31	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	47.02	47.02

[Download Data of Table SS-QC ->](#)

Table SS-BT. Concentrations of compounds in standard solution BT

№	Compound	C ^{certified} (TIS), µg/g	C ^{certified} (TIS), g/100L AA	C ^{certified} (EIS), g/100L AA
1	acetaldehyde	2.11	0.50	0.45
2	ethyl acetate	2.93	0.69	0.63
3	acetal	1.71	0.41	0.37
4	methanol	4.65	1.10	1.00
5	2-butanol	0.00	0.00	0.00
6	n-propanol	0.00	0.00	0.00
7	2-methyl-1-propanol	0.00	0.00	0.00
8	n-butanol	0.00	0.00	0.00
9	2-methyl-1-butanol	0.00	0.00	0.00
10	3-methyl-1-butanol	0.00	0.00	0.00
11	ethanol	332937.64	78927.00	78927.00
12	4-methyl-1-pentanol	198.00	46.94	46.94

[Download Data of Table SS-BT ->](#)

Table RRF. The values of $RRF^{4\text{-methyl-1-pentanol}}$ and $RRF^{ethanol}$ obtained using TIS and EIS methods

№	Compound	$RRF^{4\text{-methyl-1-pentanol}}$	$RRF^{ethanol}$
1	acetaldehyde	2.724	1.372
2	ethyl acetate	1.680	0.846
3	acetal	1.396	0.703
4	methanol	2.328	1.171
5	2-butanol	1.191	0.601
6	n-propanol	1.253	0.632
7	2-methyl-1-propanol	1.074	0.541
8	n-butanol	1.092	0.550
9	2-methyl-1-butanol	0.962	0.485
10	3-methyl-1-butanol	1.012	0.510
11	ethanol	1.984	1.000
12	4-methyl-1-pentanol	1.000	0.504

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