BÜCHI Extraction System **B-811**

A Comprehensive Guide to Evaluate your Heating Steps

This guide line will help you to set the right heating steps for your extraction procedure. Step prediction is possible based on the enthalpy of vaporization of a compound. Empirically we found the following correlation shown in figure 1. The equation is valid for a boiling point up to 150°C and vaporization enthalpies up to 45 kJ/mol.

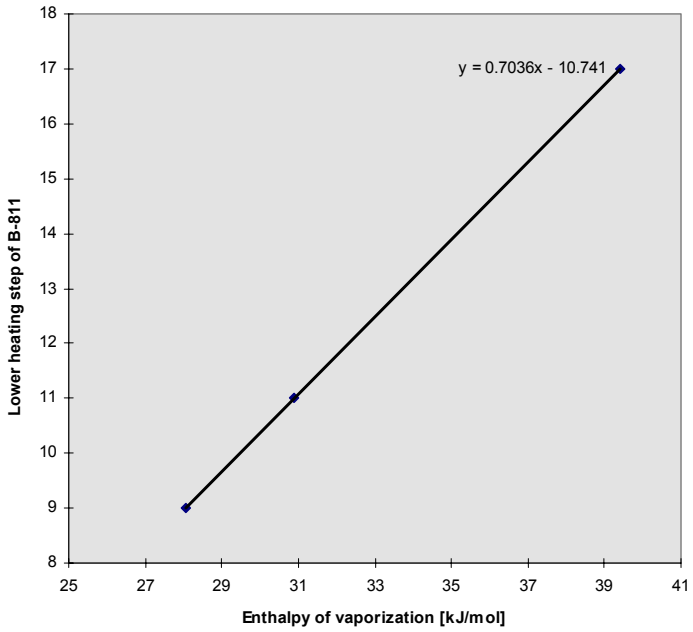

Fig. 1: Correlation of enthalpy of vaporization [kJ/mol] and lower heating step of the BÜCHI Extraction System B-811

Equation 1 describes the mathematical correlation:

(1) **$LH = 0.7036 \cdot \Delta H(T_b) - 10.741$**

LH	lower heating step
$\Delta H(T_b)$	enthalpy of vaporization on boiling point [kJ/mol]

Now you can predict the lower heating step for various solvents. However, you also have to set the upper heating step when using the extraction modes Soxhlet Warm or Hot Extraction. Calculating the maximal upper heating step for your extraction problem, you can use the following equation 2:

(2) **$UH(max) = T_b/20$**

UH(max)	maximal upper heating step
T_b	boiling point of solvent point [°C]

Table 2 shows settings for various solvents predicted with equation 1 and 2. [1]

Legend

T_b [°C]:	Boiling point of the solvent at normal pressure [2]
$\Delta H(T_b)$:	Enthalpy of vaporization of the solvent at boiling point [3]
LH:	Lower heating step
UH(max):	Maximal upper heating step

[1] It should be mentioned that from case to case, the practical heating steps may differ from the predicted ones.
[2] Ref.: Handbook of Chemistry and Physics, 71st Edition, 1990-1991, CRC Press, 6-86 - 6-93
[3] Ref.: Handbook of Chemistry and Physics, 71st Edition, 1990-1991, CRC Press, 6-86 - 6-93

Solvent	T_b [°C]	$\Delta H(T_b)$	LH	UH (max)
Acetone	56.1	30.9	11	3
Allyl bromide	70.1	30.24	11	4
Benzene	80.1	30.72	11	5
Bis(ethoxymethyl)ether	140.6	36.17	15	8
Bromoethane	38.5	27.04	8	2
Butyl propyl ether	118.1	33.72	13	6
Butanenitrile	117.6	33.68	13	6
Butyl ethanoate (butyl acetate)	126.1	36.28	15	7
Butyl ethyl ether	92.3	31.63	12	5
Butyl vinyl ether	94	31.58	11	5
Butylamine	77.1	31.81	12	4
Butylethylamine	107.5	33.97	13	6
Butyl ethyl sulfide	144.3	37.01	15	8
Carbon disulfide	46.3	26.74	8	3
Chlorobenzene	131.8	35.19	14	7
Chloropentafluorobenzene	118.1	34.76	14	6
cis-1,2-Dimethylcyclohexane	129.8	33.47	13	7
cis-1,3-Dimethylcyclohexane	120.11	32.91	12	7
cis-1,3-Dimethylcyclopentane	90.8	30.4	11	5
cis-1,4-Dimethylcyclohexane	124.4	33.28	13	7
Cyclobutanecarbonitrile	149.6	36.88	15	8
Cyclohexane	80.8	29.97	10	5
Cyclohexanethiol	158.9	37.06	15	8
Cyclohexene	83.1	30.46	11	5
Cyclohexylami'ne	134	36.14	15	7
Cyclopentane	49.3	27.3	8	3
Cyclopentanone	130.6	36.35	15	7
Cyclopropanecarbonitrile	135.1	35.55	14	7
Cyclopropyl methyl ketone	111.3	34.07	13	6
Decane	174.1	38.75	17	9
Di-sec-butyl ether	121.1	34.06	13	7
Di-tert-butyl ether	107.3	32.15	12	6
Di-tert-butyl sulfide	149.1	33.26	13	8
Dibromomethane	97	32.92	12	5
Dichloromethane	39.9	28.06	9	2
Diethyl ether	34.5	26.52	8	2
Diethyl sulfide	92.1	31.77	12	5
Diethylamine	55.6	29.06	10	3
Diisopropyl ether	68.4	29.1	10	4
Diisopropyl sulfide	120.1	33.8	13	7
Diisopropylami'ne	84	30.4	11	5
Diketene	126.1	36.8	15	7
Dimethly formamide	152.8	42.24	19	8
Dimethyl disulfide	109.8	33.78	13	6
Dimethyl sulfide	37.4	27	8	2
Dipropyl ether	90	31.31	11	5
Dipropyl sulftde	142.9	36.6	15	8

Solvent	T_b [°C]	$\Delta H(T_b)$	LH	UH (max)
Dipropylamine	109.3	33.47	13	6
Ethanenitrile (acetonitrile)	81.6	29.75	10	5
Ethanethiol	35.1	26.79	8	2
Ethanoic acid (acetic acid)	118	23.7	6	6
Ethanol	78.4	38.56	16	4
Ethyl 2,2-dimethylpropanoate	118.4	34.51	14	6
Ethyl 2-methylpropanoate	110.1	33.67	13	6
Ethyl butanoate	121.5	35.47	14	7
Ethyl chloroethanoate	144.3	40.43	18	8
Ethyl ethanoate (ethyl acetate)	77.1	31.94	12	4
Ethyl methanoate (ethyl formate)	54.4	29.91	10	3
Ethyl methyl sulfide	66.6	29.53	10	4
Ethyl pentanoate	146.1	36.96	15	8
Ethyl pentyl ether	117.6	34.41	13	6
Ethylbenzene	136.1	35.57	14	7
Ethylcyclobutane	70.81	28.67	9	4
Ethylcyclohexane	131.91	34.04	13	7
Ethylcyclopentane	103.5	31.96	12	6
Ethylisopropylamine	69.6	29.94	10	4
Fluorobenzene	84.8	31.19	11	5
Furan	31.4	27.1	8	2
Heptane	98.5	31.77	12	5
Hexafluorobenzene	80.1	31.66	12	5
Hexane	68.8	28.85	10	4
Hexyl methyl ether	126.1	34.93	14	7
Hexylamine	132.8	36.54	15	7
Isobutyl bromide	91.1	31.33	11	5
Isobutyl chloride	68.5	29.22	10	4
Isobutyl iodide	121.1	33.54	13	7
Isobutylamine	67.6	30.61	11	4
Isohexane	60.3	27.79	9	4
Isopropyl methyl ether	30.8	26.05	8	2
Isopropyl methyl sulfide	84.8	30.71	11	5
Isopropyl propyl sulfide	132.1	35.11	14	7
Isopropylamine	31.8	27.83	9	2
Isopropylmethylamine	50.4	28.71	9	3
Isopropylpropylamine	96.9	32.14	12	5
Iodoethane	72.5	29.44	10	4
Isopropyicyclopentane	126.5	33.56	13	7
Methanoic acid (formic acid)	100.6	22.69	5	6
Methanol	64.6	35.21	14	4
Methyl 2,2-dimethylpropanoate	101.1	33.42	13	6
Methyl chloroethanoate	129.5	39.23	17	7
Methyl cyclobutanecarboxylate	135.5	37.13	15	7
Methyl cyclopropanecarboxylate	114.9	35.25	14	6
Methyl dichloroethanoate	142.9	39.28	17	8
Methyl ethahoate (methyl acetate)	57	30.32	11	3

Solvent	T_b [°C]	$\Delta H(T_b)$	LH	UH (max)
Methyl hexanoate	149.5	38.55	16	8
Methyl methanoate (methyl forrnate)	31.6	27.92	9	2
Methyl pentanoate	127.4	35.36	14	7
Methyl pentyl ether	98.9	32.02	12	5
Methyl pentyl sulfide	145.1	37.41	16	8
Methyl phenyl ether	153.6	38.97	17	8
Methyl propanoate	79.8	32.24	12	4
Methyl propyl ether	39.1	26.75	8	2
Methyl propyl sulfide	95.6	32.08	12	5
Methylcyclohexane	101	31.27	11	6
Methylcyclopentane	71.9	29.08	10	4
Methylhydrazine	90.9	36.12	15	5
Methyloxirane	34.61	27.35	9	2
Nitromethane	101.31	33.99	13	6
Nonane	150.9	36.91	15	8
Octadecafluorooctane	105.9	33.38	13	6
Octane	125.6	34.41	13	7
Oxetane	47.6	28.67	9	3
Pentafluorobenzene	85.8	32.15	12	5
Pentanenitrile	141.3	36.09	15	8
Pentylamine	104.3	34.01	13	6
Propanal	48	28.31	9	3
Propanenitrile	97.9	31.81	12	5
Propyl methanoate (propyl formate)	80.9	33.61	13	5
Propyl propanoate	122.5	35.54	14	7
Propylamine	47.3	29.55	10	3
Propylcyclopentane	131	34.7	14	7
Pyridine	115.3	35.09	14	6
Pyrimidine	123.8	43.09	20	7
Pyrrole	129.9	38.75	17	7
Pyrrolidine	86.6	33.01	12	5
sec-Butyl alcohol	99.6	40.75	18	5
sec-Butyl bromide	91.4	30.77	11	5
sec-Butyl chloride	68.3	29.17	10	4
sec-Butyl iodide	120.1	33.27	13	7
sec-Butylamine	63	29.92	10	4
Spiropentane	39	26.76	8	2
tert-Butyl alcohol	82.4	39.07	17	5
tert-Butyl bromide	73.3	29.23	10	4
tert-Butyl chloride	50.9	27.55	9	3
tert-Butyl iodide	100.1	31.43	11	6
tert-Butylamine	44.1	28.27	9	3
Tetrachloroethylene	121	34.68	14	7
Tetrachloromethane	76.8	29.82	10	4
Tetrahydrofuran	66	29.81	10	4
Tetranitromethane	126.1	40.74	18	7

Solvent	T_b [°C]	$\Delta H(T_b)$	LH	UH (max)
Thiacyclobutane	95	32.32	12	5
Thiacyclopentane	121.1	34.66	14	7
Thiophene	84.1	31.48	11	5
trans-1,2-Dimethylcyclohexane	123.5	32.96	12	7
trans-1,3-Dimethylcyclohexane	124.5	33.39	13	7
trans-1,4-Dimethylcyclohexane	119.4	32.56	12	6
trans-3-Pentenenitrile	142.6	37.09	15	8
Tribromomethane	149.1	39.66	17	8
Trichloroethylene	87.3	31.4	11	5
Trichloromethane	61.1	29.24	10	4
Triethylamine	89	31.01	11	5
(Trifluoromethyl)benzene	102.1	32.63	12	6
1,1 -Dichloroethane	57.3	28.85	10	3
1,1 -Dichloroethylene	31.6	26.14	8	2
1,1 -Dimethylethyl ethanoate	95.1	33.07	13	5
1,1, 1 -Trichloroethane	74.1	29.86	10	4
1,1, 1 -Trichlorotrifluoroethane	46.1	26.85	8	3
1,1,2,2-Tetrachloroethane	146.3	37.64	16	8
1,1,2-Trichloroethane	113.8	34.82	14	6
1,1,2-Trichlorotrifluoroethane	47.6	27.04	8	3
1,1-Dimethylcyclohexane	119.6	32.51	12	6
1,2-Dibromoethane	131.6	34.77	14	7
1,2-Dibromopropane	141.9	35.61	14	8
1,2-Dichlorobutane	124.1	33.9	13	7
1,2-Dichloroethane	83.5	31.98	12	5
1,2-Dichlorohexafluoropropane	34.1	26.28	8	2
1,2-Diethoxyethane	119.4	36.28	15	6
1,2-Difluorobenzene	94	32.21	12	5
1,2-Dimethoxyethane	84.9	32.42	12	5
1,2-Dimethylbenzene	144.5	36.24	15	8
1,2-Ethanediamine	117	37.98	16	6
1,2-Ethanedithiol	146.1	37.93	16	8
1,3-Dichloropropane	120.9	35.18	14	7
1,3-Difluorobenzene	82.6	31.1	11	5
1,3-Dimethylbenzene	139.1	35.66	14	7
1,3-Dioxane	106.1	34.37	13	6
1,3-Propanediamine	139.8	40.85	18	7
1,4-Difluorobenzene	88.9	31.77	12	5
1,4-Dimethylbenzene	138.4	35.67	14	7
1,4-Dimethylbenzene	138.4	35.67	14	7
1,4-Dioxane	101.4	34.16	13	6
1-Bromobutane	101.6	32.51	12	6
1-Chlorobutane	78.6	30.39	11	4
1-Chlorohexane	135	35.67	14	7
1-Hexanol	157.41	44.5	21	8
1-Iodobutane	130.6	34.66	14	7
1-Iodopropane	102.6	32.08	12	6

Solvent	T_b [°C]	$\Delta H(T_b)$	LH	UH (max)
1-Methylbicyclo(3, 1,0)hexane	93.11	31.07	11	5
1-Pentene	30	25.2	7	2
1-Propanethiol	67.8	29.54	10	4
1-Propanoi	97.1	41.44	18	5
1 -Bromopropane	71.1	29.84	10	4
1 -Butanethiol	98.5	32.23	12	5
1 -Butanol	117.8	43.29	20	6
1 -Chloropropane	46.5	27.18	8	3
1 -Ethyl-1 -methylcyclopentane	121.6	33.2	13	7
1 -Fluorooctane	142.4	40.43	18	8
1 -Octene	121.3	34.07	13	7
1 -Octyne	126.3	35.83	14	7
2-Methyl-I-butene	31.1	25.5	7	2
2-Methylnonane	167.1	38.23	16	9
2-Methylpropanenitrile	103.9	32.39	12	6
2-Methylpyridine	129.5	36.17	15	7
2-Methylthiophene	112.6	33.9	13	6
2-Methythexane	90.1	30.62	11	5
2-Octyne	137.6	37.26	15	7
2-Propanethiol	52.6	27.91	9	3
2-Propanol	82.3	39.85	17	5
2-Propanone (acetone)	56.1	29.1	10	3
2 2,4-Trimethylpentane	99.3	30.79	11	5
2,2,3-Trimethylbutane	80.9	28.9	10	5
2,2,3-Trimethylpentane	109.9	31.94	12	6
2,2,4,4-Tetramethylpentane	122.4	32.51	12	7
2,2,4-Trimethyl-3-pentanone	135.1	35.64	14	7
2,2,5-Trimethylhexane	124.1	33.65	13	7
2,2-Dimethyl-3-pentanone	125.6	36.09	15	7
2,2-Dimethylbutane	49.8	26.31	8	3
2,2-Dimethylhexane	108.9	32.07	12	6
2,2-Dimethylpentane	79.3	29.23	10	4
2,2-Dimethylpropanenitrile	106.1	32.4	12	6
2,3,4,5,6-Pentafluorotoluene	117.5	34.75	14	6
2,3,4-Trimethylpentane	113.5	32.36	12	6
2,3,5-Trimethylhexane	131.4	34.43	13	7
2,3-Dihydrothiophene	112.1	33.24	13	6
2,3-Dimethyl-2-butene	73.3	29.64	10	4
2,3-Dimethylbutane	58	27.38	9	3
2,3-Dimethylhexane	115.6	33.17	13	6
2,3-Dimethylpentane	89.8	30.46	11	5
2,4-Dimethyl-3-pentanone	125.4	34.64	14	7
2,4-Dimethylhexane	109.5	32.51	12	6
2,4-Dimethylpentane	80.6	29.55	10	5
2,4-Pentanone	138	34.3	13	7
2,5-Dihydrothiophene	122.4	34.83	14	7
2,5-Dimethylhexane	109.1	32.54	12	6

Solvent	T_b [°C]	$\Delta H(T_b)$	LH	UH (max)
2,6-Dimethylpyridine	144.1	37.46	16	8
2:3,3-Trimethylpentane	114.8	32.12	12	6
2-Bromopropane	59.5	28.33	9	3
2-Butanethiol	85	30.59	11	5
2-Butanone	79.6	31.3	11	4
2-Ethoxyethanol	135	39.22	17	7
2-Hexanoi	139.9	41.01	18	7
2-Hexanone	127.6	36.35	15	7
2-Iodopropane	89.5	30.68	11	5
2-Methoxyethanol	124.1	37.54	16	7
2-Methyl-1 -propanethiol	88.5	31.01	11	5
2-Methyl-1 -propanol	108	41.82	19	6
2-Methyl-2-butene	38.6	26.31	8	2
2-Methyl-2-pentanol	121.1	39.59	17	7
2-Methyl-2-propanethiot	64.3	28.45	9	4
2-Methyl-3-pentanone	113.5	33.84	13	6
2-Methyldecane	189.3	40.25	18	10
2-Methylheptane	117.6	33.26	13	6
3,3-Diethylpentane	146.3	34.61	14	8
3,3-Dimethyl-2-butanone	106.1	33.39	13	6
3,3-Dimethylhexane	112	32.31	12	6
3,3-Dimethylpentane	86.1	29.62	10	5
3,4-Dimethylhexane	117.8	33.24	13	6
3-Ethyl-2-methylpentane	115.6	32.93	12	6
3-Ethyl-3-methylpentane	118.3	32.78	12	6
3-Ethylpentane	93.5	31.12	11	5
3-Ethythexane	118.6	33.59	13	6
3-Hexanone	123.6	35.36	14	7
3-Methyl-2-pentanone	117.5	34.16	13	6
3-Methylbutanenitrile	127.5	35.1	14	7
3-Methylheptane	119	33.66	13	6
3-Methylhexane	91.9	30.89	11	5
3-Methylpentane	63.3	28.06	9	4
3-Methylpyridine	144.1	37.35	16	8
3-Methylthiophene	115.5	34.24	13	6
3-Octyne	133.1	36.94	15	7
4-Fluorotoluene	116.6	34.08	13	6
4-Methyl-2-pentanone	116.3	34.49	14	6
4-Methyl-I-pentanol	151.9	44.46	21	8
4-Methylpyridine	145.4	37.51	16	8
4-Methylthiazole	133.3	37.58	16	7
4-Methytheptane	117.8	33.35	13	6
4-Octyne	131.6	36	15	7

Tab. 2: Predicted heating steps of the B-811 for various solvents