# TDTS 20

# Confirming sorbent tube retention volumes and checking for analyte breakthrough

*It is recommended that this Application Note is read in conjunction with Application Note TDTS 5 (Advice on sorbent selection, tube conditioning, tube storage and air sampling).*

## Introduction

Information on how to determine sorbent tube retention volumes, breakthrough volumes and safe sampling volumes is presented in Application Note TDTS 5 and in various international standard methods for thermal desorption, *e.g.* EN ISO 16017-1, Annexes A and B. However, as sorbent tubes age it is possible for retention volumes to fall, risking breakthrough of the most volatile target compounds. It is also possible for breakthrough volumes to fall under extreme environmental conditions (*e.g.* high humidity and high temperature), though the impact of such effects varies significantly for different sorbents.

This Application Note describes a simple procedure for checking analyte breakthrough prior to or during field monitoring, using pairs of tubes linked together in series. This guidance also complies with recommendations in standard thermal desorption methods for air monitoring.

## Field validation of quantitative retention during sampling

As a routine check of pumped tube retention during field air monitoring studies, two identical, conditioned sorbent tubes should be linked together in series using an inert stainless steel union with combined PTFE ferrules (part number C-UN010). The sampling end of the back-up tube should be connected to the outlet end of the front (sampling) tube. The sampling pump is attached to the exhaust end of the back-up tube. At least one such tube pair should be deployed in all routine monitoring exercises and, in large scale studies, it is recommended that at least one in ten monitoring locations are sampled using such tube pairs.

After monitoring, the back-up tubes should be analysed in the same analytical sequence as all the sampling tubes and study blanks.

- If the mass of one or more target analytes on the back-up tube is >5% of the mass on the front sampling tube, *breakthrough* of that compound or compounds can be said to have occurred. The amount can quantified by adding the mass of analyte measured on the back-up tube to that determined on the front sampling tube.
- If the mass of one or more target analytes on the back-up tube is >10% of the mass on the front sampling tube, breakthrough of that compound or compounds is significant, and data for any such compounds should not be viewed as quantitative.

## Extended checks of breakthrough and other tube performance indicators

After a batch of tubes has been used extensively (*e.g.* 20 field monitoring exercises or thermal cycles) a representative number of tubes from that batch should be more stringently checked for breakthrough. In this case it is recommended that at least six tube pairs are prepared as above and used to sample a standard or real atmosphere under conditions which are as close as possible to the worst-case real-life scenario, *i.e.* highest natural humidity, highest ambient temperature and highest expected VOC concentrations.

The sampling points of all the tube pairs should placed close together to ensure that, as far as possible, they are all sampling the same atmosphere. The selected sampling location should be well ventilated. Three different pump flow rates between 10 and 200 mL/min should be used for sampling, with duplicates at each level. All the tubes should be analysed in one sequence, and the results evaluated to ensure that compound masses increase relative to the volume of air sampled and are reproducible at each volume. Selective loss of one or more analytes at higher volumes indicates breakthrough. Detection of >5% of one or more analytes on the back-up tubes can be used to confirm breakthrough.

If one or more analyte is observed to increase at a higher rate than the sample volume, this can be an indication of artefact formation or sorbent/analyte breakdown. Such effects can be caused, for example, by the air containing above-ambient concentrations of reactive gases such as ozone, or by sorbent degradation. In the latter case, the tubes would need repacking.

## Appendix – Breakthrough volumes

### Notes on the tables

- Markes has not undertaken any validation work on the following data. It is always recommended that safe sampling volumes are checked using one of the procedures outlined above
- Breakthrough volumes have been extrapolated to relate to a standard ¼″ stainless steel TD tube, packed with the typical mass of sorbent
- SSV = Safe sampling volume
- U = Unretained.

### 1. On 200 mg Carbotrap C–Carbograph 2TD at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Methane | –164 | U | — |
| Ethane | –89 | U | — |
| Propane | –42 | U | — |
| Butane | –0.5 | U | — |
| Pentane | 36 | U | — |
| Hexane | 69 | 0.3 | 0.15 |
| Heptane | 98 | 1.4 | 0.7 |
| Octane | 125 | 5.6 | 2.8 |
| Nonane | 151 | 20 | 10 |
| Decane | 174 | 100 | 50 |
| Undecane | 196 | 500 | 250 |
| Dodecane | 216 | 2600 | 1300 |
| Tridecane | 235 | 7400 | 3700 |
| Tetradecane | 254 | 22000 | 11000 |
| Pentadecane | 271 | 46000 | 23000 |
| Hexadecane | 287 | 100000 | 50000 |
| Heptadecane | 302 | 300000 | 150000 |
| Octadecane | 316 | 800000 | 400000 |
| ***Alcohols*** | | | |
| Methanol | 65 | U | — |
| Ethanol | 78 | U | — |
| Propan-1-ol | 97 | U | — |
| Butan-1-ol | 118 | U | — |
| Pentan-1-ol | 138 | 0.42 | 0.21 |
| Hexan-1-ol | 158 | 1.42 | 0.71 |
| Heptan-1-ol | 176 | 6.6 | 3.3 |
| Octan-1-ol | 195 | 16 | 8 |
| Nonan-1-ol | 213 | 40 | 20 |
| Decan-1-ol | 231 | 90 | 45 |
| Undecan-1-ol | 243 | 240 | 120 |
| Dodecan-1-ol | 259 | 800 | 400 |
| Tridecan-1-ol | — | 2000 | 1000 |
| Tetradecan-1-ol | 289 | 3200 | 1600 |
| Pentadecan-1-ol | — | 7200 | 3600 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Halogenated compounds*** | | | |
| *Monohalogenated compounds* | | | |
| Chloromethane | –24 | U | — |
| Chloroethene (Vinyl chloride) | –13 | U | — |
| 2-Chloroethyl vinyl ether | 109 | 0.1 | 0.05 |
| Chlorobenzene | 132 | 1 | 0.5 |
| *Dihalogenated compounds* | | | |
| 1,1-Dichloroethane | 57 | U | — |
| 1,2-Dichloroethane | 83 | U | — |
| 1,1-Dichloroethene | 32 | U | — |
| 1,2-Dichloroethene | 49 | U | — |
| 1,2-Dichloropropane | 95 | U | — |
| 1,3-Dichloropropene | 104–112 | U | — |
| 1,2-Dichlorobenzene | 181 | 6 | 3 |
| 1,3-Dichlorobenzene | 173 | 6 | 3 |
| 1,4-Dichlorobenzene | 174 | 6 | 3 |
| *Trihalogenated compounds* | | | |
| Bromodichloromethane | 90 | U | — |
| Dibromochloromethane | 119 | U | — |
| Chlorodifluoromethane | –41 | U | — |
| Trichloromethane | 61 | U | — |
| Tribromomethane | 149 | 0.1 | 0.5 |
| 1,1,1-Trichloroethane | 74 | U | — |
| 1,1,2-Trichloroethane | 110 | U | — |
| Trichloroethene | 87 | U | — |
| *Tetrahalogenated compounds* | | | |
| Dichlorodifluoromethane | –30 | U | — |
| Trichlorofluoromethane | 24 | U | — |
| Tetrachloromethane | 76 | U | — |
| 1,1,2,2-Tetrachloroethane | 146 | 0.2 | 0.1 |
| Tetrachloroethene | 121 | 0.4 | 0.02 |

### 2. On 200 mg Tenax TA at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Methane | –164 | U | — |
| Ethane | –89 | U | — |
| Propane | –42 | U (0.03) | — |
| Butane | –0.5 | 0.2 | 0.1 |
| Pentane | 36 | 1 | 0.5 |
| Hexane | 69 | 6.4 | 3.2 |
| Heptane | 98 | 34 | 17 |
| Octane | 125 | 160 | 80 |
| Nonane | 151 | 1400 | 700 |
| Decane | 174 | 4200 | 2100 |
| Undecane | 196 | 25000 | 12500 |
| Dodecane | 216 | 126000 | 63000 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes (continued)*** | | | |
| Tridecane | 235 | 25000 | 12500 |
| Tetradecane | 254 | 60000 | 30000 |
| Pentadecane | 271 | 114000 | 57000 |
| Hexadecane | 287 | 210000 | 105000 |
| Heptadecane | 302 | 340000 | 170000 |
| Octadecane | 316 | 560000 | 280000 |
| Nonadecane | 330 | 800000 | 400000 |
| Eicosane | 343 | $1.32 \times 10^6$ | 660000 |
| n-$C_{21}$ | 357 | $2.0 \times 10^6$ | $1.0 \times 10^6$ |
| n-$C_{22}$ | 369 | $3.2 \times 10^6$ | $1.6 \times 10^6$ |
| n-$C_{23}$ | 380 | $5.0 \times 10^6$ | $2.5 \times 10^6$ |
| n-$C_{24}$ | 391 | $8.2 \times 10^6$ | $4.1 \times 10^6$ |
| n-$C_{25}$ | 402 | $1.25 \times 10^8$ | $6.25 \times 10^6$ |
| n-$C_{26}$ | 412 | $2.5 \times 10^7$ | $1.25 \times 10^6$ |
| n-$C_{27}$ | 442 | $5.0 \times 10^7$ | $2.5 \times 10^6$ |
| n-$C_{28}$ | 432 | $1.04 \times 10^8$ | $5.2 \times 10^6$ |
| n-$C_{29}$ | 441 | $2.2 \times 10^8$ | $1.1 \times 10^8$ |
| n-$C_{30}$ | 450 | $5.0 \times 10^8$ | $2.5 \times 10^8$ |
| ***Aromatics*** | | | |
| Benzene | 80 | 12.5 | 6 |
| Toluene | 111 | 76 | 38 |
| Xylene | 138–144 | 610 | 305 |
| Ethylbenzene | 137 | 360 | 180 |
| n-Propylbenzene | 159 | 1700 | 850 |
| Isopropylbenzene | 152 | 960 | 480 |
| n-Butylbenzene | 183 | 3600 | 1800 |
| n-Hexylbenzene | 226 | 87200 | 43600 |
| Ethyltoluene | 162 | 2000 | 1000 |
| Styrene | 145 | 600 | 300 |
| Methylstyrene | 167 | 2400 | 1200 |
| Nitrobenzene | 211 | 28000 | 14000 |
| *p*-Cymene | 177 | 2600 | 1300 |
| Butylated hydroxy toluene (BHT) | 265 | 2700 | 1350 |
| Trimethylbenzene | 165–176 | 3600 | 1800 |
| *o*-Cresol | 191 | 6600 | 3300 |
| *p*-Cresol | 202 | 6200 | 3100 |
| *o*-Ethyltoluene | 164 | 2000 | 1000 |
| *m*-Ethyltoluene | 161 | 2000 | 1000 |
| *p*-Ethyltoluene | 162 | 2000 | 1000 |
| Naphthalene | 218 | 20000 | 10000 |
| Biphenyl | 256 | 63200 | 31600 |
| Phenanthrene | 340 | 112400 | 56200 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Terpenes and alkaloids*** | | | |
| Limonene | 176 | 2400 | 1200 |
| Nicotine | 247 | 20000 | 10000 |
| Geraniol | 229 | 126000 | 63000 |
| Cotinine | — | 280000 | 140000 |
| ***Alkenes*** | | | |
| But-1-ene | –6 | 0.1 | 0.05 |
| Pent-1-ene | 30 | 0.9 | 0.45 |
| Pent-2-ene | 37 | 1.2 | 0.6 |
| Hex-1-ene | 63 | 4.6 | 2.3 |
| Hex-2-ene | 68 | 6.4 | 3.2 |
| Hex-3-ene | 66 | 5.6 | 2.8 |
| Hept-1-ene | 94 | 24 | 12 |
| Oct-1-ene | 121 | 112 | 56 |
| Oct-2-ene | 123 | 164 | 82 |
| Oct-3-ene | 121 | 130 | 65 |
| Non-1-ene | — | 640 | 320 |
| Dec-1-ene | 170 | 1260 | 630 |
| Undec-1-ene | — | 2820 | 1410 |
| Dodec-1-ene | 214 | 5600 | 2800 |
| Tridec-1-ene | — | 8400 | 4200 |
| Tetradec-1-ene | — | 12600 | 6300 |
| Pentadec-1-ene | — | 20000 | 10000 |
| Hexadec-1-ene | — | 31600 | 15800 |
| Heptadec-1-ene | — | 50200 | 25100 |
| Octadec-1-ene | — | 80000 | 40000 |
| Nonadec-1-ene | — | 200000 | 100000 |
| Eicos-1-ene | — | 500000 | 250000 |
| ***Esters*** | | | |
| Methyl acetate | 57 | 1.6 | 0.8 |
| Ethyl acetate | 71 | 54 | 27 |
| Propyl acetate | 102 | 36 | 18 |
| Isopropyl acetate | 90 | 12 | 6 |
| n-Butyl acetate | 126 | 170 | 85 |
| Isobutyl acetate | 115 | 265 | 132.5 |
| *tert*-Butyl acetate | 98 | 176 | 88 |
| Pentyl acetate | 149 | 940 | 470 |
| Hexyl acetate | 172 | 9000 | 4500 |
| Methyl acrylate | 81 | 13 | 6.5 |
| Ethyl acrylate | 100 | 48 | 24 |
| Methyl methacrylate | 100 | 55 | 27.5 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Glycol ethers*** | | | |
| Methoxyethanol | 125 | 6 | 3 |
| Ethoxyethanol | 136 | 10 | 5 |
| Butoxyethanol | 170 | 70 | 35 |
| 2-(2-Butoxyethoxy)-ethanol | – | 50200 | 25100 |
| Methoxypropanol | 118 | 27 | 13.5 |
| Methoxyethyl acetate | 145 | 16 | 8 |
| Ethoxyethyl acetate | 156 | 30 | 15 |
| Butoxyethyl acetate | 92 | 300 | 150 |
| ***Aldehydes*** | | | |
| Acetaldehyde | 20 | 0.1 | 0.05 |
| Propanal | 48 | 1 | 0.5 |
| 2-Methylpropanal | 63 | 3.4 | 1.7 |
| Butanal | 75 | 6 | 3 |
| 3-Methylbutanal | 91 | 13 | 6.5 |
| Pentanal | 103 | 22 | 11 |
| Hexanal | 131 | 100 | 50 |
| Heptanal | 153 | 700 | 350 |
| Octanal | 169 | 2500 | 1250 |
| Nonanal | 191 | 12600 | 6300 |
| 2-Methylcyclohexane carboxaldehyde | – | 500 | 250 |
| 3-Methylcyclohexane carboxaldehyde | – | 600 | 300 |
| 4-Methylcyclohexane carboxaldehyde | – | 800 | 400 |
| Furfural | 162 | 600 | 300 |
| ***Ketones*** | | | |
| Acetone | 56 | 1.2 | 0.6 |
| Butan-2-one (Methyl ethyl ketone) | 80 | 6.4 | 3.2 |
| Pentan-2-one | 102 | 36 | 18 |
| Pentan-3-one | 102 | 40 | 20 |
| 4-Methylpentan-2-one (Methyl isobutyl ketone) | 116 | 52 | 26 |
| Hexan-2-one | 128 | 200 | 100 |
| Heptan-2-one | 151 | 1000 | 500 |
| Heptan-3-one | 147 | 800 | 400 |
| Heptan-4-one | 144 | 700 | 350 |
| Octan-2-one | 173 | 4000 | 2000 |
| Octan-3-one | 167 | 1160 | 580 |
| Nonan-2-one | 195 | 10000 | 5000 |
| Nonan-4-one | 187 | 6400 | 3200 |
| Cyclohexanone | 155 | 340 | 170 |
| 3,5,5-Trimethylcyclohex-2-en-1-one | 214 | 11200 | 5600 |
| Benzaldehyde | 179 | 220 | 110 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alcohols*** | | | |
| Methanol | 65 | U | – |
| Ethanol | 78 | 0.4 | 0.2 |
| Propan-1-ol | 97 | 2.2 | 1.1 |
| Propan-2-ol | 82 | 1 | 0.5 |
| 2-Methylpropan-2-ol | 83 | 10 | 5 |
| Butan-1-ol | 118 | 10 | 5 |
| Butan-2-ol | 108 | 5.6 | 2.8 |
| 2-Methylbutan-1-ol | 129 | 16 | 8 |
| 3-Methylbutan-1-ol | 130 | 32 | 16 |
| 2-Methylbutan-2-ol | 101 | 0.2 | 0.1 |
| Dimethylaminoethanol | 133 | 36 | 18 |
| Pentan-1-ol | 138 | 76 | 38 |
| Pentan-2-ol | 119 | 34 | 17 |
| Pentan-3-ol | 115 | 9 | 4.5 |
| Hexan-1-ol | 158 | 360 | 180 |
| Heptan-1-ol | 176 | 2000 | 1000 |
| Octan-1-ol | 195 | 2800 | 1400 |
| Nonan-1-ol | 213 | 17800 | 8900 |
| Decan-1-ol | 231 | 56200 | 28100 |
| Undecan-1-ol | 243 | 141600 | 70800 |
| Dodecan-1-ol | 259 | 280000 | 140000 |
| Tridecan-1-ol | – | 400000 | 200000 |
| Tetradecan-1-ol | 289 | 640000 | 320000 |
| Pentadecan-1-ol | – | $1.12 \times 10^6$ | 560000 |
| Hexadecan-1-ol | – | $1.80 \times 10^6$ | 900000 |
| Heptadecan-1-ol | – | $3.56 \times 10^6$ | $1.78 \times 10^6$ |
| Octadecan-1-ol | – | $7 \times 10^6$ | $3.5 \times 10^6$ |
| Nonadecan-1-ol | – | $2 \times 10^7$ | $1 \times 10^7$ |
| Eicosan-1-ol | – | $5.62 \times 10^7$ | $2.81 \times 10^6$ |
| Docosan-1-ol | – | $4 \times 10^8$ | $2 \times 10^8$ |
| Phenol | 182 | 480 | 240 |
| *o*-Cresol | 191 | 6600 | 3300 |
| *p*-Cresol | 201 | 6200 | 3100 |
| ***Glycols*** | | | |
| Ethylene glycol | 197 | 7 | 3.5 |
| Propane-1,2-diol | 186 | 20 | 10 |
| Butane-1,3-diol | 203 | 157 | 78.5 |
| (2-Hydroxyethoxy)-ethan-2-ol (Diethylene glycol) | 245 | 1260 | 630 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Halogenated compounds*** | | | |
| *Monohalogenated compounds* | | | |
| Chloromethane | –24 | U | – |
| Chloroethane | 12 | 0.8 | 0.4 |
| Chloroethene (Vinyl chloride) | –13 | 0.1 | 0.05 |
| 2-Chloroethyl vinyl ether | 109 | 40 | 20 |
| Chlorobenzene | 131 | 52 | 26 |
| *Dihalogenated compounds* | | | |
| Dichloromethane | 40 | 0.9 | 0.45 |
| 1,1-Dichloroethane | 57 | 2.2 | 1.1 |
| 1,2-Dichloroethane | 84 | 10.8 | 5.4 |
| 1,1-Dichloroethene | 32 | 0.8 | 0.4 |
| 1,2-Dichloroethene | 49 | 1.8 | 0.9 |
| 1,2-Dichloropropane | 95 | 16 | 8 |
| 1,3-Dichloropropene | 104–112 | 30 | 15 |
| 1,2-Dichlorobenzene | 181 | 660 | 330 |
| 1,3-Dichlorobenzene | 173 | 540 | 270 |
| 1,4-Dichlorobenzene | 174 | 58 | 290 |
| *Trihalogenated compounds* | | | |
| Bromodichloromethane | 90 | 18 | 9 |
| Dibromochloromethane | 119 | 63 | 31.5 |
| Chlorodifluoromethane | –41 | U | – |
| Trichloromethane (Chloroform) | 61 | 3.8 | 1.9 |
| Tribromomethane (Bromoform) | 149 | 200 | 100 |
| 1,1,1-Trichloroethane | 74 | 2.2 | 1.1 |
| 1,1,2-Trichloroethane | 114 | 68 | 34 |
| Trichloroethene | 87 | 11 | 5.5 |
| *Tetrahalogenated compounds* | | | |
| Dichlorodifluoromethane | –30 | U | – |
| Trichlorofluoromethane | 24 | 0.4 | 0.2 |
| Tetrachloromethane | 76 | 12.4 | 6.2 |
| Tetrachloromethane | 76 | 4.2 | 2.1 |
| 1,1,1,2-Tetrachloroethane | 130 | 156 | 78 |
| 1,1,2,2-Tetrachloroethane | 146 | 340 | 170 |
| Tetrachloroethene | 121 | 96 | 48 |
| ***Acids*** | | | |
| Acetic acid | 118 | 1.1 | 0.55 |
| Propanoic acid | 141 | 6.4 | 3.2 |
| Butanoic acid | 164 | 28 | 14 |
| Pentanoic acid | 186 | 140 | 70 |
| Hexanoic acid | 205 | 620 | 310 |
| ***Acid anhydrides*** | | | |
| Maleic anhydride | 202 | 176 | 88 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Amines*** | | | |
| Methylamine | –6 | 0.1 | 0.05 |
| Ethylamine | 17 | 0.9 | 0.45 |
| n-Propylamine | 48 | 3.2 | 1.6 |
| n-Butylamine | 77 | 13 | 6.5 |
| *sec*-Butylamine | 83 | 4.6 | 2.3 |
| Isobutylamine | 68 | 5 | 2.5 |
| *tert*-Butylamine | 44 | U | – |
| n-Pentylamine | 104 | 52 | 26 |
| Isopentylamine | 95 | 26 | 13 |
| n-Hexylamine | 129 | 200 | 100 |
| Cyclohexylamine | 133 | 180 | 90 |
| n-Heptylamine | 154 | 1000 | 500 |
| n-Octylamine | 178 | 3600 | 1800 |
| n-Nonylamine | 202 | 9000 | 4500 |
| n-Decylamine | 216 | 28200 | 14100 |
| Pyridine | 116 | 16 | 8 |
| Aniline | 183 | 440 | 220 |
| Benzylamine | 184 | 1000 | 500 |

### 3. On 200 mg Tenax GR at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Methane | –164 | U | – |
| Ethane | –89 | U | – |
| Propane | –42 | U | – |
| Butane | –0.5 | U (0.08) | – |
| Pentane | 36 | 0.34 | 0.17 |
| Hexane | 69 | 1.3 | 0.65 |
| Heptane | 98 | 6 | 3 |
| Octane | 125 | 18 | 9 |
| Nonane | 151 | 50 | 25 |
| Decane | 174 | 240 | 120 |
| Dodecane | 216 | 820 | 410 |
| Tetradecane | 254 | 2400 | 1200 |
| Hexadecane | 287 | 9400 | 4700 |
| Octadecane | 316 | 40000 | 20000 |
| Eicosane | 343 | 170000 | 85000 |
| ***Aldehydes*** | | | |
| Propanal | 48 | 0.6 | 0.3 |
| 2-Methylpropanal | 63 | 1.2 | 0.6 |
| Butanal | 75 | 1.9 | 0.95 |
| 3-Methylbutanal | 91 | 4.4 | 2.2 |
| Pentanal | 103 | 5 | 2.5 |
| Hexanal | 131 | 14 | 7 |
| Heptanal | 153 | 56 | 28 |
| Octanal | 169 | 120 | 60 |
| Nonanal | 191 | 160 | 160 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Ketones*** | | | |
| Acetone | 56 | 0.7 | 0.35 |
| Butan-2-one (Methyl ethyl ketone) | 80 | 2.4 | 1.2 |
| Pentan-2-one | 102 | 4.8 | 2.4 |
| Pentan-3-one | 102 | 5 | 2.5 |
| Hexan-2-one | 128 | 14 | 7 |
| 2-Methylcyclohexanone | – | 24 | 12 |
| 3-Methylcyclohexanone | – | 12 | 6 |
| 4-Methylcyclohexanone | – | 13 | 6.5 |
| Heptan-2-one | 151 | 40 | 20 |
| Heptan-3-one | 147 | 39 | 19.5 |
| Heptan-4-one | 144 | 32 | 16 |
| Octan-2-one | 173 | 100 | 50 |
| Octan-3-one | 167 | 42 | 21 |
| Nonan-2-one | 195 | 300 | 150 |
| Nonan-5-one | 186 | 280 | 140 |
| ***Alcohols*** | | | |
| Methanol | 65 | U | – |
| Ethanol | 78 | U (0.16) | – |
| Propan-1-ol | 97 | 0.6 | 0.16 |
| propan-2-ol | 82 | 0.32 | 0.3 |
| Butan-1-ol | 118 | 2 | 0.55 |
| Butan-2-ol | 98 | 1.1 | 1 |
| Pentan-1-ol | 138 | 4.6 | 1.6 |
| Pentan-2-ol | 119 | 3.2 | 2.3 |
| Hexan-1-ol | 158 | 20 | 10 |
| Heptan-1-ol | 180 | 46 | 23 |
| Octan-1-ol | 195 | 100 | 50 |
| Nonan-1-ol | 213 | 170 | 85 |
| Decan-1-ol | 231 | 400 | 200 |
| Undecan-1-ol | 243 | 600 | 300 |
| Dodecan-1-ol | 259 | 1200 | 600 |
| Tridecan-1-ol | – | 2000 | 1000 |
| Tetradecan-1-ol | 289 | 3600 | 1800 |
| Pentadecan-1-ol | – | 4400 | 2200 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Halogenated compounds*** | | | |
| *Monohalogenated compounds* | | | |
| Chloromethane | –24 | U | – |
| Chloroethane | 12 | 0.1 | 0.05 |
| Chloroethene (Vinyl chloride) | –13 | U | – |
| 2-Chloroethyl vinyl ether | 109 | 6 | 3 |
| Chlorobenzene | 132 | 20 | 10 |
| *Dihalogenated compounds* | | | |
| Dichloromethane | 40 | 0.5 | 0.25 |
| 1,1-Dichloroethane | 57 | 0.8 | 0.4 |
| 1,2-Dichloroethane | 83 | 2.4 | 1.2 |
| 1,1-Dichloroethene | 32 | 0.5 | 0.25 |
| 1,2-Dichloroethene | 49 | 0.6 | 0.3 |
| 1,2-Dichloropropane | 95 | 2.2 | 1.1 |
| 1,3-Dichloropropene | 104–112 | 4 | 2 |
| 1,2-Dichlorobenzene | 181 | 160 | 80 |
| 1,3-Dichlorobenzene | 173 | 120 | 60 |
| 1,4-Dichlorobenzene | 174 | 140 | 70 |
| *Trihalogenated compounds* | | | |
| Bromodichloromethane | 90 | 2 | 1 |
| Dibromochloromethane | 119 | 10 | 5 |
| Chlorodifluoromethane | –41 | U | – |
| Trichloromethane (Chloroform) | 61 | 1.2 | 0.6 |
| Tribromomethane (Bromoform) | 149 | 40 | 20 |
| 1,1,1-Trichloroethane | 74 | 1.8 | 0.9 |
| 1,1,2-Trichloroethane | 110 | 6 | 3 |
| Trichloroethene | 87 | 3.4 | 1.7 |
| *Tetrahalogenated compounds* | | | |
| Dichlorodifluoromethane | –30 | U | – |
| Trichlorofluoromethane | – | 0.1 | 0.05 |
| Tetrachloromethane | 76 | 2 | 1 |
| 1,1,2,2-Tetrachloroethane | 146 | 38 | 19 |
| Tetrachloroethene | 121 | 7.6 | 3.8 |
| ***Amines*** | | | |
| n-Butylamine | 77 | 2.4 | 1.2 |
| *sec*-Butylamine | 83 | 1 | 0.5 |
| Isobutylamine | 68 | 1.3 | 0.65 |
| *tert*-Butylamine | 44 | U | – |
| n-Pentylamine | 104 | 14 | 7 |
| Isopentylamine | 95 | 4 | 2 |
| n-Hexylamine | 129 | 40 | 20 |
| Cyclohexylamine | 133 | 5 | 2.5 |
| n-Heptylamine | 154 | 70 | 35 |
| n-Octylamine | 178 | 170 | 85 |
| n-Decylamine | 216 | 400 | 200 |
| Benzylamine | 184 | 70 | 35 |

### 4. On 200 mg Carbotrap/Carbograph 1TD/Carbopack B at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Methane | –164 | U | — |
| Ethane | –89 | U | — |
| Propane | –42 | U | — |
| Butane | –0.5 | U | — |
| Pentane | 36 | 1.2 | 0.6 |
| Hexane | 69 | 16 | 8 |
| Heptane | 98 | 90 | 45 |
| Octane | 125 | 1500 | 750 |
| Nonane | 151 | 14000 | 7000 |
| Decane | 174 | 200000 | 100000 |
| Undecane | 96 | 600000 | 300000 |
| Dodecane | 216 | $1.6 \times 10^6$ | 800000 |
| ***Alcohols*** | | | |
| Methanol | 65 | U | — |
| Ethanol | 78 | U | — |
| Propan-1-ol | 97 | 0.64 | 0.32 |
| Butan-1-ol | 118 | 6 | 3 |
| Pentan-1-ol | 138 | 20 | 10 |
| Hexan-1-ol | 158 | 60 | 30 |
| Heptan-1-ol | 176 | 180 | 90 |
| Octan-1-ol | 180 | 600 | 300 |
| Nonan-1-ol | 213 | 3000 | 1500 |
| Decan-1-ol | 231 | 6000 | 3000 |
| ***Halogenated compounds*** | | | |
| *Monohalogenated compounds* | | | |
| Chloromethane | –24 | U | — |
| Chloroethene (Vinyl chloride) | –13 | U | — |
| 2-Chloroethyl vinyl ether | 109 | 2.6 | 1.3 |
| Chlorobenzene | 132 | 20 | 10 |
| *Dihalogenated compounds* | | | |
| Dichloromethane | 40 | 0.04 | 0.02 |
| 1,1-Dichloroethane | 57 | 0.2 | 0.1 |
| 1,2-Dichloroethane | 83 | 0.3 | 0.15 |
| 1,1-Dichloroethene | 32 | 0.1 | 0.05 |
| 1,2-Dichloroethene | 49 | 0.2 | 0.1 |
| 1,2-Dichloropropane | 95 | 1.2 | 0.6 |
| 1,3-Dichloropropene | 104–112 | 1.3 | 0.65 |
| 1,2-Dichlorobenzene | 181 | 102 | 51 |
| 1,3-Dichlorobenzene | 173 | 102 | 51 |
| 1,4-Dichlorobenzene | 174 | 102 | 51 |
| ***Halogenated compounds (continued)*** | | | |
| *Trihalogenated compounds* | | | |
| Dibromochloromethane | 119 | 1.5 | 0.75 |
| Trichloromethane (Chloroform) | 61 | 0.2 | 0.1 |
| Tribromomethane (Bromoform) | 149 | 3.8 | 1.9 |
| 1,1,1-Trichloroethane | 74 | 0.6 | 0.3 |
| 1,1,2-Trichloroethane | 110 | 1.6 | 0.8 |
| Trichloroethene | 87 | 1.6 | 0.8 |
| *Tetrahalogenated compounds* | | | |
| Dichlorodifluoromethane | –30 | U | — |

### 5. On 300 mg Carbopack X

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| Carbon disulfide[a] | 46 | 6.5 | 3 |
| Buta-1,3-diene | –4 | >25 | >17 |
| Benzene | 80 | 10800 | 5400 |

[a] At 30°C, 80% relative humidity.

### 6. On 300 mg Chromosorb 106

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Pentane | 35 | 11.2 | 56 |
| Hexane | 69 | 60 | 30 |
| Heptane | 98 | 325 | 162 |
| Octane | 125 | 2076 | 1038 |
| Nonane | 151 | 14000 | 7000 |
| Decane | 174 | 74000 | 37000 |
| ***Aromatics*** | | | |
| Benzene | 80 | 53 | 26 |
| Toluene | 111 | 165 | 82 |
| Xylene | 138–144 | 1554 | 777 |
| Ethylbenzene | 137 | 730 | 365 |
| Trimethylbenzene | 165–176 | 5650 | 2825 |
| ***Esters*** | | | |
| Methyl acetate | 58 | 5.2 | 2.6 |
| Ethyl acetate | 71 | 39 | 19.5 |
| Propyl acetate | 102 | 297 | 148.5 |
| Isopropyl acetate | 90 | 147 | 73.5 |
| n-Butyl acetate | 126 | 1460 | 730 |
| Isobutyl acetate | 115 | 880 | 440 |
| *tert*-Butyl acetate | 98 | 327 | 163.5 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Glycol ethers*** | | | |
| Methoxyethanol | 125 | 9.6 | 4.8 |
| Ethoxyethanol | 136 | 150 | 75 |
| Methoxyethyl acetate | 145 | 1720 | 860 |
| Ethoxyethyl acetate | 156 | 8100 | 4050 |
| ***Ketones*** | | | |
| Acetone | 56 | 2.9 | 1.45 |
| Butan-2-one (Methyl ethyl ketone) | 80 | 21 | 10.5 |
| 4-Methylpentan-2-one (Methyl isobutyl ketone) | 118 | 490 | 245 |
| ***Alcohols*** | | | |
| Ethanol | 78 | 2.4 | 1.2 |
| Propan-1-ol | 97 | 17 | 8.5 |
| Propan-2-ol | 82 | 9 | 4.5 |
| Butan-1-ol | 118 | 96 | 48 |
| Butan-2-ol | 108 | 60 | 30 |
| ***Halogenated compounds*** | | | |
| Tetrachloromethane | 76 | 44 | 22 |
| 1,2-Dichloroethane | 84 | 34 | 17 |
| 1,1,1-Trichloroethane | 74 | 17 | 8.5 |

### 7. On 500 mg PoraPak N

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Pentane | 35 | 8.2 | 4.1 |
| Hexane | 69 | 32 | 16 |
| Heptane | 98 | 90 | 45 |
| ***Aromatics*** | | | |
| Benzene | 80 | 52 | 26 |
| Pyridine | 116 | 390 | 195 |
| ***Ketones*** | | | |
| Butan-2-one (Methyl ethyl ketone) | 80 | 95 | 47.5 |
| ***Alcohols*** | | | |
| Ethanol | 78 | 7.5 | 3.75 |
| Propan-1-ol | 97 | 40 | 20 |
| Butan-1-ol | 118 | 10 | 5 |
| Butan-2-ol | 108 | 5.6 | 2.8 |
| Octan-1-ol | 180 | 2800 | 1400 |
| Phenol | 182 | 480 | 240 |
| ***Acids*** | | | |
| Acetic acid | 116 | 97 | 48.5 |
| ***Nitriles*** | | | |
| Acetonitrile | 82 | 7 | 3.5 |
| Acrylonitrile | 82 | 7 | 3.5 |
| Propionitrile | 97 | 23 | 11.5 |

### 8. On 300 mg UniCarb

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| Butane | –0.5 | 1640 | 820 |
| Pentane | 35 | 63000 | 31500 |
| Hexane | 69 | $3.9 \times 10^6$ | $1.95 \times 10^6$ |
| Benzene | 80 | $1 \times 10^6$ | 500000 |
| Dichloromethane | 40 | 395 | 197 |
| 1,1,1-Trichloroethane | 74 | 17600 | 8800 |
| Methanol | 65 | 264 | 132 |
| Ethanol | 78 | 6900 | 3450 |
| Carbon disulfide[a] | 46 | 26 | 13 |

[a] At 30°C, 80% relative humidity.

### 9. On 600 mg Carbosieve SIII at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Alkanes*** | | | |
| Methane | –164 | U (0.05) | — |
| Ethane | –89 | 0.7 | — |
| Propane | –42 | 5.1 | 2.55 |
| Butane | –0.5 | 37.8 | 18.9 |
| Pentane | 36 | 360 | 180 |
| Hexane | 69 | 3000 | 1500 |
| Heptane | 98 | 6000 | 3000 |

### 10. On 500 mg Carboxen 569 at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Aromatics*** | | | |
| Benzene | 80 | 42.5 | 21.25 |
| Toluene | 111 | 1350 | 675 |
| Ethylbenzene | 137 | 1250 | 625 |
| Isopropylbenzene | 152 | 3750 | 1875 |
| Trimethylbenzene | 165–176 | 3750 | 1875 |
| Xylene | 138–144 | 5500 | 2750 |
| Benzaldehyde | 179 | 6000 | 3000 |
| *p*-Cymene | 177 | 10000 | 5000 |
| Propylbenzene | 159 | 11000 | 5500 |
| ***Terpenes*** | | | |
| Limonene | 176 | 8000 | 4000 |
| Terpinene | 182 | 10000 | 5000 |

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| ***Aldehydes*** | | | |
| Propanal | 48 | 1.2 | 0.6 |
| Butanal | 75 | 2.6 | 1.3 |
| 2-Methylpropanal | 63 | 4.25 | 2.125 |
| Pentanal | 103 | 35 | 17.5 |
| Hexanal | 131 | 600 | 300 |
| Heptanal | 153 | 10500 | 5250 |
| Octanal | 169 | 30000 | 15000 |
| Nonanal | 191 | 90000 | 45000 |
| ***Ketones*** | | | |
| Acetone | 56 | 3.5 | 1.75 |
| Butan-2-one (Methyl ethyl ketone) | 80 | 2 | 1 |
| Pentan-2-one | 102 | 10.5 | 5.25 |
| Pentan-3-one | 102 | 20 | 10 |
| Hexan-2-one | 128 | 400 | 200 |
| 2-Methylcyclohexanone | — | 65000 | 32500 |
| 3-Methylcyclohexanone | — | 400 | 200 |
| 4-Methylcyclohexanone | — | 400 | 200 |
| Heptan-2-one | 151 | 60000 | 30000 |
| Heptan-3-one | 147 | 60000 | 30000 |
| Heptan-4-one | 144 | 60000 | 30000 |
| Octan-3-one | 167 | 35000 | 17500 |
| ***Halogenated compounds*** | | | |
| Tribromomethane (Bromoform) | 149 | 1000 | 500 |
| 1,1,2,2-Tetrachloroethane | 146 | 2000 | 1000 |
| ***Amines*** | | | |
| n-Butylamine | 77 | 5.5 | 2.75 |
| *sec*-Butylamine | 83 | 5.2 | 2.6 |
| Isobutylamine | 68 | 4.1 | 2.05 |
| *tert*-Butylamine | 44 | 1.6 | 0.8 |
| n-Pentylamine | 104 | 95 | 47.5 |
| Isopentylamine | 95 | 10.5 | 5.25 |
| n-Hexylamine | 129 | $3 \times 10^6$ | $1.5 \times 10^6$ |
| Benzylamine | 184 | 60000 | 30000 |
| ***Other*** | | | |
| Carbon disulfide[a] | 46 | 72 | 36 |

[a] At 30°C, 80% relative humidity.

### 11. On 350 mg Carbograph 5TD at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| Buta-1,3-diene | –4 | ~10 | ~7 |

### 12. On 600 mg Molecular sieve 13X at 20°C

| Compound | b.p. (°C) | Retention volume (L) | SSV (L) |
|---|---|---|---|
| Buta-1,3-diene | –4 | >100 | >70 |

### 13. Breakthrough volumes for water

It is important to use at least twice the volumes below when purging water from the sorbent bed, to ensure complete elution. It is also important that the water is kept in the gas phase.

| Sorbent | Temp. (°C) | Breakthrough volume | |
|---|---|---|---|
| | | Manufacturers' data (mL/g)[a] | Extrapolated to typical mass of sorbent in ¼″ stainless steel tube (mL) |
| Carbotrap C | 20 | 25 | 5 |
| Tenax TA | 20 | 65 | 13 |
| | 40 | — | 7[a] |
| | 60 | — | 3.6[a] |
| Tenax GR | 20 | 47 | 9.4 |
| Carbotrap | 20 | 39 | 7.8 |
| Carboxen 569 | 20 | 60 | 12 |
| Carbosieve SIII | 20 | 320 | 64 |

[a] For 200 mg Tenax TA.

## Trademarks

UniCarb™ is a trademark of Markes International Ltd, UK.

Carbograph™ is a trademark of LARA s.r.l., Italy.

Carbopack™ is a trademark of Supelco Inc., USA.

Carbosieve™ is a trademark of Supelco Inc., USA.

Carbotrap® is a registered trademark of Sigma-Aldrich Co. LLC, USA.

Carboxen™ is a trademark of Supelco Inc., USA.

Chromosorb® is a registered trademark of Manville Corporation, USA.

PoraPak™ is a trademark of Waters Associates Inc., USA.

Version 8
June 2012