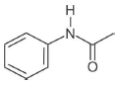
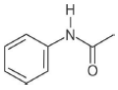
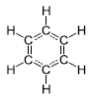
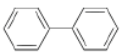
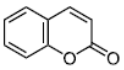
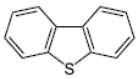
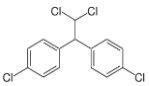
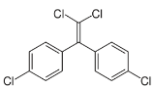
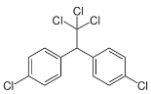
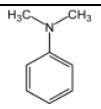
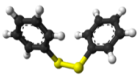
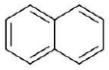
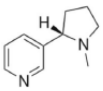
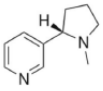
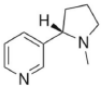
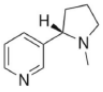
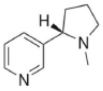
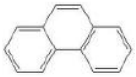
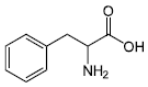
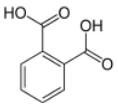
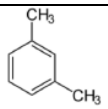
Version 18 October 2025 **Aromatic compounds** formula, CAS #, purity, amount, type of packaging, price in US $	Structure	$\delta^{2}H$ (or δD) (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}C$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}N$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}O$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)
Acetanilide #1, C_8H_9NO, CAS # 103-84-4, in glass vial, 5 g US $250, 2 g US $150		not determined (contains exchangeable hydrogen)	**-29.53** ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	**+1.18** ± 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined
Acetanilide #3, C_8H_9NO, CAS # 103-84-4, in glass vial, 2 g US $250		not determined (contains exchangeable hydrogen)	**-29.50** ± 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	**+40.57** ± 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined
Benzene #1, C_6H_6, CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US $250		**-62.4** ± 1.1 ‰ from -60.9 to -63.7 ‰ n = 5	**-27.68** ± 0.01 ‰ from -27.67 to -27.69 ‰ n = 4	not applicable	not applicable
Benzoic acid #A, $C_7H_6CO_2$, CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	**-28.81** ‰ Coplen et al., 2006 DOI: 10.1021/ac052027c	not applicable	**+23.14** ± 0.19 ‰ Brand et al., 2009 DOI: 10.1002/rcm.3958
Benzoic acid #B, $C_7H_6CO_2$, enriched in ^{18}O, CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	**-28.85** ‰ Coplen et al., 2006 DOI: 10.1021/ac052027c	not applicable	**+71.28** ± 0.36 ‰ Brand et al., 2009 DOI: 10.1002/rcm.3958
Biphenyl, $C_{12}H_{10}$, 99.94 %, CAS # 92-52-4, 10 mg in crimp-sealed glass vial, US $250		**-41.2** ± 1.3 ‰ from -39.5 to -42.9 ‰ n = 6	**-25.16** ± 0.01 ‰ from -25.15 to -25.17 ‰ n = 4	not applicable	not applicable
Coronene, $C_{24}H_{12}$, 99 %, CAS # 191-07-1, at least 5 mg in crimp-sealed glass vial, US $250		**-48.3** ± 0.9 ‰ from -47.3 to -49.3 ‰ n = 4	**-26.81** ± 0.04 ‰ from -26.77 to -26.85 ‰ n = 4	not applicable	not applicable
Coumarin, $C_9H_6O_2$, ≥99.5 %, CAS # 91-64-5, 100 mg in crimp-sealed glass vial, US $250		**+82.3** ± 1.2 ‰ from +80.9 to +83.7 ‰ n = 4	**-35.60** ± 0.01 ‰ from -35.59 to -35.61 ‰ n = 3	not applicable	not determined
Dibenzothiophene, $C_{12}H_8S$, 99.4 %, CAS # 132-65-0, at least 10 mg in crimp-sealed glass vial, US $250		**+84.9** ± 1.8 ‰ from +82.4.2 to +87.5 ‰ n = 6	**-27.68** ± 0.01 ‰ from -27.66 to -27.69 ‰ n = 4	not applicable	not applicable
p, p'-Dichlorodiphenyldichloro-ethane, $C_{14}H_{10}Cl_4$, p,p'-DDD, CAS # 72-54-8, 98 %, 10 mg in crimp-sealed glass vial, US $250		**+72.0** ± 1.2 ‰ from +70.1 to +73.5 ‰ n = 5	**-27.86** ± 0.02 ‰ from -27.84 to -27.88 ‰ n = 4	not applicable	not applicable
p, p'-Dichlorodiphenyldichloro-ethene, $C_{14}H_8Cl_4$, p,p'-DDE, CAS # 72-55-9, 99 %, 10 mg in crimp-sealed glass vial, US $250		**-81.8** ± 2.0 ‰ from -78.3 to -83.9 ‰ n = 6	**-23.61** ± 0.02 ‰ from -23.59 to -23.63 ‰ n = 4	not applicable	not applicable
Dichlorodiphenyltrichloroethane, $C_{14}H_9Cl_5$, 4,4'-DDT, CAS # 50-29-3, 10 mg in crimp-sealed glass vial, US $250		**-13.9** ± 0.8 ‰ from -13.0 to -15.0 ‰ n = 4	**-28.54** ± 0.02 ‰ from -28.52 to -28.55 ‰ n = 4	not applicable	not applicable
N,N-Dimethylaniline, $C_8H_{11}N$, CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US $250		**-48.2** ± 2.2 ‰ from -45.2 to -51.0 ‰ n = 5	**-23.79** ± 0.01 ‰ from -23.78 to -23.80 ‰ n = 4	**-1.15** ± 0.03 ‰ from -1.10 to -1.18 ‰ n = 4	not applicable
Diphenyldisulfide, $C_{12}H_{10}S_2$, Ph_2S_2, CAS # 882-33-7, 99 %, 10 mg in crimp-sealed glass vial, US $250		**-148.4** ± 4.0 ‰ from -142.4 to -152.4 ‰ n = 5	**-25.63** ± 0.02 ‰ from -25.61 to -25.66 ‰ n = 4	not applicable	not determined
9-Ethylcarbazole, $C_{14}H_{13}N$, ≥99.5 %,CAS # 86-28-2, ≥200 mg in crimp-sealed glass vial, US $250		**-102.0** ± 1.1 ‰ from -100.6 to -103.6 ‰ n = 7	**-25.36** ± 0.02 ‰ from -25.35 to -25.39 ‰ n = 5	**+3.93** ± 0.06 ‰ from +3.87 to +4.00 ‰ n = 5	not applicable
Naphthalene, $C_{10}H_8$, ≥99.7 %, CAS # 91-20-3, 10 mg in crimp-sealed glass, US $250		**-58.6** ± 1.0 ‰ from -57.4 to -59.5 ‰ n = 5	**-26.12** ± 0.02 ‰ from -26.10 to -26.14 ‰ n = 4	not applicable	not applicable

Version 18 October 2025 **Aromatic compounds** formula, CAS #, purity, amount, type of packaging, price in US $	Structure	$\delta^{2}H$ (or δD) (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}C$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}N$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}O$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)
Nicotine #1, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**-29.98** ± 0.01 ‰ from -29.97 to -30.00 ‰ n = 5	**-5.82** ± 0.05 ‰ from -5.75 to -5.88 ‰ n = 4	not applicable
Nicotine #2, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**+7.72** ± 0.02 ‰ from +7.68 to +7.75 ‰ n = 7	**-5.94** ± 0.15 ‰ from -5.72 to -6.18 ‰ n = 7	not applicable
Nicotine #3, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**-30.05** ± 0.02 ‰ from -30.03 to -30.07 ‰ n = 7	**+33.62** ± 0.18 ‰ from +33.40 to +33.83 ‰ n = 7	not applicable
Nicotine #4, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**-2.06** ± 0.02 ‰ from -2.04 to -2.08 ‰ n = 5	**+15.49** ± 0.13 ‰ from +15.31 to +15.68 ‰ n = 7	not applicable
Nicotine #5, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		**-161.3** ± 1.7 ‰ from -159.2 to -164.6 ‰ n = 10	**-29.63** ± 0.01 ‰ from -29.61 to -29.65 ‰ n = 5	**-6.03** ± 0.04 ‰ from -5.97 to -6.08 ‰ n = 5	not applicable
Phenanthrene, $C_{14}H_{10}$, ≥99.5 %, CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US $250		**-84.1** ± 1.3 ‰ from -82.8 to -86.2 ‰ n = 6	**-25.39** ± 0.03 ‰ from -25.36 to -25.42 ‰ n = 6	not applicable	not applicable
L-Phenylalanine, $C_9H_{11}NO_2$, ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US $250		not determined (contains exchangeable hydrogen)	**-11.20** ± 0.02 ‰ from -11.19 to -11.23 ‰ n = 6	**+1.70** ± 0.06 ‰ from +1.64 to +1.77 ‰ n = 5	not determined
Phthalic acid #2, $C_8H_6O_4$, CAS # 88-99-3, $\delta^{2}H$ measured in Na-phthalate to exclude carboxyl hydrogen. $\delta^{13}C$ measured in free acid. 3 g in glass vial, US $250		**-81.9** ± 1.2 ‰ from -81.8 to -83.0 ‰ n = 4	**-29.98** ± 0.01 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined
Pyrazine, $C_4H_4N_2$, CAS # 290-37-9, at least 20 mg in sealed glass capillary, US $250		**-31.8** ± 1.7 ‰ from -29.4 to -34.2 ‰ n = 6	not determined	**+1.39** ± 0.04 ‰ from +1.34 to +1.43 ‰ n = 4	not applicable
Pyrene, $C_{16}H_{10}$, CAS # 129-00-0, 98.5 %, 30 mg in crimp-sealed glass vial, US $250		**-108.1** ± 1.3 ‰ from -106.5 to -109.8 ‰ n = 5	**-24.52** ± 0.01 ‰ from -24.51 ‰ to -24.52 ‰ n = 5	not applicable	not applicable
Toluene #1, C_7H_8, CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US $250		**-73.2** ± 2.1 ‰ from -70.8 to -76.5 ‰ n = 5	**-25.02** ± 0.02 ‰ from -25.00 to -25.04 ‰ n = 4	not applicable	not applicable
Toluene #2, C_7H_8, CAS # 108-88-3, 99.5 %, 0.5 mL sealed under argon in glass ampoule, US $250		**-76.1** ± 0.7 ‰ from -74.8 to -80.1 ‰ n = 54	**-25.03** ± 0.02 ‰ from -24.99 to -25.06 ‰ n = 37	not applicable	not applicable
***m*-Xylene #1**, C_8H_{10}, CAS # 108-38-3, ≥99 %, 1 mL sealed under argon in glass ampoule, US $250		**-58.6** ± 1.3 ‰ from -57.1 to -60.5 ‰ n = 5	**-27.27** ± 0.01 ‰ from -27.26 to -27.28 ‰ n = 4	not applicable	not applicable