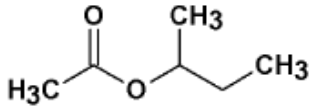
Substance name: sec-butyl acetate

CAS: 105-46-4 MW: 116.16 gm/mole

Synonyms: 2-butyl acetate; acetic acid, secondary butyl ester; acetic acid, 1-methylpropyl ester
Molecular formula: $C_6H_{12}O_2$ Structural formula:



ppm to mg/M^3 conversion factors at 20 ºC and 760 mm/Hg: 1 ppm = 4.83 mg/m^3
Physical characteristics at room temp:

boiling point 234 ºF
melting point -107 ºF
vapor pressure 19 mmHg
solubility 30 gm/l
density 0.87 gm/cm^3
Log P_{ow} 1.51 (calculated)

Special physical characteristics if any:

colorless with fruity odor

Flammability and other hazards:

flash point 88 ºF (closed cup); 62 ºF (open cup)

Uses/applications:

It is usually found in as a component in paints and in the production of paper coatings.

Major commercial form(s):

Estimated uses: nitrocellulose-based lacquers 63%, exports 27%, ink solvent 5%, adhesives solvent 2%, and other solvent uses 3%. As a lacquer solvent it is used in wooden furniture and auto top-coat applications. Other uses may include solvent in the production of airplane dopes, extraction solvent in the manufacture of penicillin, synthetic flavoring ingredient used in producing banana, pear, pineapple and berry flavors, solvent for fats, waxes, camphor, gums, resins, lacquer stains, ester-soluble dyes and cellulose esters. In commercial grade it has been used in the manufacturing of vinyl resins, and preservation of foodstuffs. Other reported uses include photographic film manufacturing, in nail polish removers, other products for manicure, and as a flavoring agent in the cosmetics industry. It occurs naturally in bananas and other related fruits, and it is created during fermentation processes.

Odor Thresholds:

Detection: 0.31 ppm; Recognition: 0.68 ppm (AIHA 1997).

Metabolism:

All butyl acetates are absorbed by the lung, the gastrointestinal tract and to a smaller extent through the skin. Once absorbed, sec-butyl acetate is hydrolysed by unspecific esterases to acetic acid and sec-butanol, which is further metabolized to ethyl methyl ketone and ten excreted either by exhalation or in the urine. Dahl *et al* (1987) measured the hydrolysis rates of all four butyl acetate isomers using esterases from a rat S9-mix. Steric factors at the site of hydrolysis such as degree of branching clearly contributed to the velocity of the reaction: *n*-butyl acetate: 77 ± 3 nmol/mg protein, isobutyl acetate: 67 ± 3 nmol/mg protein, sec-butyl acetate: 62 ± 3 nmol/mg protein and *tert*-butyl acetate: 42 ± 2 nmol/mg protein. For comparison purposes, the partition coefficients for isobutyl acetate in rats for several tissues (liver: 5.06, kidney: 4.08, brain: 2.65, muscle: 2.12 and fat: 21.3) and the blood/air partition coefficient (880).

Organizational sources and recommendations:

Source and date	Findings/Recommendations	Basis/source/ref(s)	Discussion and Assessment
Cal/OSHA Title 8	PEL 150 ppm; STEL 200 ppm		

NIOSH REL (1992)	TWA 150 ppm; STEL 200 ppm		
ACGIH TLV (2015)	TWA 50 ppm; STEL 150 ppm	Eye and upper respiratory tract irritation.	
MAK (current)	TWA 100 ppm		
Washington State OSHA	TWA 150 ppm; STEL 200 ppm		

Peer-reviewed journal articles and other studies:

Author/date	Study type	Results	Discussion and Assessment
Unpublished (Roudabush, 1970)	Acute inhalation study in rats.	No lethality from exposure to 3,500 ppm sec-butyl acetate for 6 hours. All rats exposed to 24,000 ppm for 4 hours died.	
Greim 1999	Acute oral study in rats.	The LD50 is 3,200 ppm.	
Abraham 1996	Acute inhalation study in anosmic humans where sec-butyl acetate exposure lasted two seconds.	A threshold value of 3,950 ppm for nasal irritation was determined.	
Cox 1975	No data was reported for sec-butyl acetate, however its main metabolite sec-butanol, tested in a two-generation oral study in rats.	No adverse effects on fertility at oral doses of approximately 4,500 mg/kg/day.	
Nelson 1989	No data on the developmental toxicity of sec-butyl acetate were available. However, inhalation studies with its main metabolite sec-butanol were performed in rats at concentrations of 0, 3500, 5000, and 7000 ppm.	Exposure on gd 1–19 (7 hours/day) resulted in an increased number of resorptions at 7,000 ppm. Furthermore, exposure to sec-butanol produced decreased fetal body weights and a reduced number of live fetuses at ≥ 5,000 ppm. Maternal toxicity manifested in reduced food consumption and decreased weight gain of the dams at all concentrations tested. At ≥ 5,000 ppm, narcosis of the dams occurred.	For sec-butanol, a NOAEC of 3,500 ppm was determined for developmental toxicity and the NOAEC for maternal toxicity was below 3,500 ppm.
Cox 1975	An oral two-generation reproductive toxicity study.	No developmental effects occurred in two filial generations (F1, F2) at approximately 1,500 mg/kg/day sec-butanol (NOAEL).	

Other Studies

Skin Absorption*:* reported to be absorbed epicutaneously by humans (Spasovski and Bencev 1971), however, a low permeability constant (1.6 ± 0.1 g/m²/hour) was reported in living human skin (Ursin 1995). And the acute toxicity of *n*-butyl acetate is considerably lower after dermal exposure than after oral exposure. Thus, no "skin" notation is proposed.

Sensitization: no data was reported on sensitization of sec-butyl acetate.

Genotoxicity Summary: No relevant data was reported on sec-butyl acetate. The genotoxic activities of metabolites *sec*-butanol and methyl ethyl ketone were tested in a study by Brooks *et al* (1988). Both *sec*-

butanol and the ketone gave negative results in an Ames test (TA98, TA100, TA1535, TA1537, TA1538), in a yeast mitotic gene conversion assay (JD1) and in cultured mammalian cells (rat liver cells, Chinese hamster ovary (CHO) cells). Furthermore, an Ames test with *Salmonella typhimurium* (TA98, TA100, TA1535, TA1537 and TA1538), performed by von der Hude *et al* (1988) gave negative results for acetic acid. Therefore, a genotoxic potential of *sec*-butyl acetate is unlikely.

The ACGIH TLV for acetates reported the acute irritancy of sec-butyl acetate to be less than n-butyl acetate, however, the data supporting this was unpublished. Another author reported less irritation for those acetates with lower boiling points (von Oettingen, 1960). This aligns with nasal irritation data published for many different organic molecules of differing boiling point: higher boiling point equals higher irritation.

HEAC Health-based Assessment and Recommendation

n-Butyl acetate, sec-butyl acetate and isobutyl acetate have structural similarities and a common metabolic pathway. The main critical effect is irritation, which is common to all three acetates. These common toxicological properties has been used to justify the same OEL for all three compounds by numerous standard-setting bodies (ACGIH TLV, SCOEL, etc.). Therefore, the n-butyl acetate data was used to establish a recommended PEL and STEL. The critical effect, irritation in humans, is based upon the LOAEC of 150 ppm in the study by Iregren et al 1993. Due to the exposure duration of 4 hours, a safety factor of 3 is justified for deriving a recommended OEL. An OEL of 50 ppm is proposed for all three butyl acetates to protect workers against systemic and local toxic effects during an 8-hour exposure.

A STEL of 150 ppm is recommended to avoid possible irritating effects reported in case and human exposure studies. sec-Butyl acetate was not sensitizing to the skin after dermal exposure of either humans or animals, nor is the permeability through human skin high enough to warrant a 'skin' notation.

CERS Usage information:

	Butyl Acetate Users in CERS *(n)* Average Daily Amount (gal)			
SIC Code	**n-**	**isobutyl**	**tert-**	**sec-**
	(130)	*(9)*	*(108)*	*(1)*
10-19	23.7	-	161.8	-
20-29	46.6	-	849.0	-
30-39	33.8	1.2	159.6	0.03
40-49		-	232.7	-
50-59	12423.1	5782.7	1651.1	-
70-79	29.4	-	46.1	-
80-99	4.5	5.3	0.4	-

Measurement information

OSHA Method 1009 (fully validated) uses a charcoal tube (or organic vapor monitor), a flowrate of 0.05 lpm, a volume range of 0.75 to 12 liters, and a GC-FID analytical method with an estimated reliable quantitation limit of 38.9 parts per billion (.0389 ppm).

NIOSH Method 1450 uses a charcoal tube (or organic vapor monitor), a GC-FID, and provides an estimated detection limit of 0.9 ug per sample. The range studied was 14-440 ug per sample. With a maximum 10L sample this would yield 0.29 to 9.26 ppm range.

Based on this information, there are no anticipated concerns with analytical feasibility to 50 ppm.

References

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