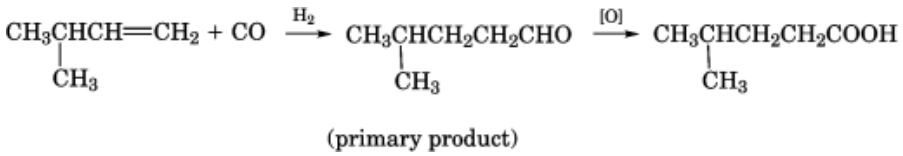
Kirk-Othmer Encyclopedia of Chemical Technology.

CARBOXYLIC ACIDS, BRANCHED-CHAIN ACIDS

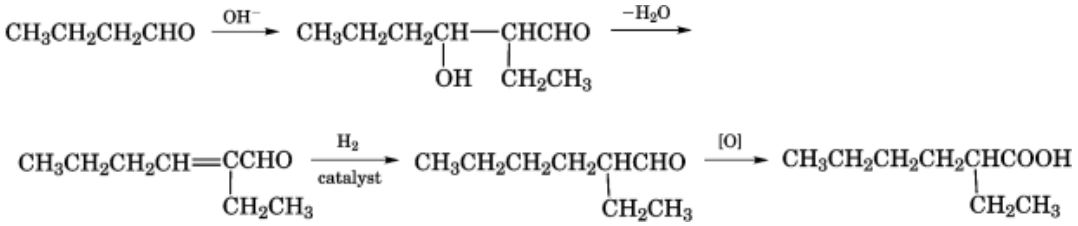
Branched-chain acids contain at least one branching alkyl group attached to the carbon chain, which causes the acid to have different physical, and in some cases different chemical, properties than their corresponding straight-chain isomers. For example, stearic acid has a melting point of about 69°C, whereas isostearic acid has a melting point of about 5°C. Some properties of commercial branched-chain acids are shown in Table 1 (1, 2).

Manufacturing procedures for most branched-chain acids are well known. For example, oxo process acids are manufactured from branched-chain olefins using hydroformylation followed by oxidation (3) (see Oxo process).



(primary product)

Neo acids are prepared from selected olefins using carbon monoxide and acid catalyst (4) (see Carboxylic acids, trialkylacetic acids). 2-Ethylhexanoic acid is manufactured by an aldol condensation of butyraldehyde followed by an oxidation of the resulting aldehyde (5). Isopalmitic acid[4669-02-7] is probably made by an aldol reaction of octanal.



Isostearic acid is produced from dimerization and reduction of monomeric acids (6).

Branched-chain acids have a wide variety of industrial uses as paint driers (7), vinyl stabilizers (8), and cosmetic products (9). Cobalt and manganese salts of 2-ethylhexanoic acid and neodecanoic acid are used as driers for paint, varnishes, and enamels; lithium, magnesium, calcium, and aluminum salts of 2-ethylhexanoic acid are used in the formation of greases and lubricants (see Driers and metallic soaps). Derivatives of isostearic acid have been used as pour point depressants in two-cycle engine oils, as textile lubricants, and in cosmetic formulations. Further industrial applications can be found (10).

Table 1. Properties and Prices of Branched-Chain Acids

Branched-chain acid (common name)	CAS Registry Number	Molecular weight	Boiling point, °C[a]	Melting point, °C	Approximate price, $/kg[b]	Producers in the United States
2-methylpropanoic (isobutyric) acid	[79-31-2]	88	155	−46.1	1.70	Hoechst, Eastman
2-methylbutanoic (isopentanoic) acid	[116-53-0]	102	180.3	−48	1.56	Union Carbide
3-methylbutanoic (isovaleric) acid	[503-74-2]	102	175–176.5	ca 30	4.73	Hoechst
2, 2-dimethylpropanoic (neopentanoic) acid	[75-98-9]	102	163–165	34.4	2.51	Exxon
2-ethylhexanoic acid	[149-57-5]	144	224–230	<70	1.52	Eastman, Union Carbide
mixed isomers (isononanoic) acid	[26896-18-4]	158	232–246	ca 70	1.69	Hoechst
2, 2-dimethyloctanoic (neodecanoic) acid	[129662-90-6]	172	147–150[c]	<40	1.96	Exxon
mixed isomers (isostearic) acid	[2724-58-5]	284	192–204[d]	ca 7	2.53	Emery, Union Camp

[a] At 101.3 kPa[e] unless otherwise indicated.
[b] In 1990, bulk, fob.
[c] At 20 kPa[e].
[d] At 5 kPa[e].
[e] To convert kPa to mm Hg, multiply by 7.5.

The hazards of handling branched-chain acids are similar to those encountered with other aliphatic acids of the same molecular weight. Eye and skin contact as well as inhalation of vapors of the shorter-chain acids should be avoided.

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ROBERT W. JOHNSON JR.
ROBERT R. CANTRELL
Union Camp Corporation

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