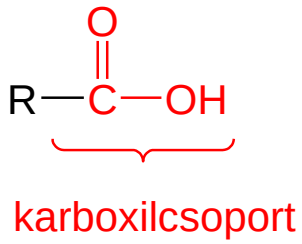
KARBONSAVAK



Példák

A) Nyílt láncú telített monokarbonsavak (zsírsavak)

"alkánsav" pl. metánsav, etánsav, propánsav...
(nem használjuk)

Homológ sor

HCOOH hangyasav	$CH_3CH_2CH_2CH_2COOH$ valeriánsav
CH_3COOH ecetsav	$CH_3CH_2CH_2CH_2CH_2COOH$ kapronsav
CH_3CH_2COOH propionsav	$CH_3(CH_2)_{14}COOH$ palmitinsav
$CH_3CH_2CH_2COOH$ vajsav	$CH_3(CH_2)_{16}COOH$ szterarinsav

B) Nyílt láncú telített dikarbonsavak

"alkándisav" pl. etándisav, propándisav...

$HOOC—COOH$
oxálsav

$HOOC—CH_2—COOH$
malonsav

$HOOC—(CH_2)_2—COOH$
borostyánkősav

$HOOC—(CH_2)_3—COOH$
glutársav

$HOOC—(CH_2)_4—COOH$
adipinsav

C) Telítetlen karbonsavak

$CH_2{=}CH—COOH$
propénsav
akrilsav

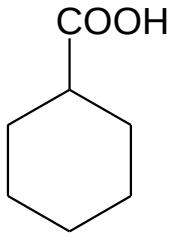
$CH_2{=}C(CH_3)—COOH$
2-metilpropénsav
metakrilsav

$CH—(CH_2)_7—COOH$
$\|$
$CH—(CH_2)_7—CH_3$
olajsav
(cisz)

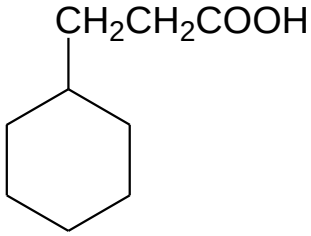
$CH—COOH$
$\|$
$CH—COOH$
maleinsav
(cisz)

$HOOC—CH$
$\|$
$CH—COOH$
fumársav
(transz)

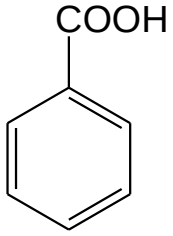
D) Gyűrűs karbonsavak



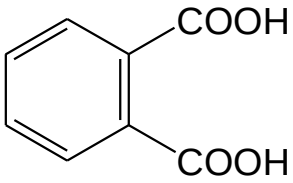
ciklohexánkarbonsav



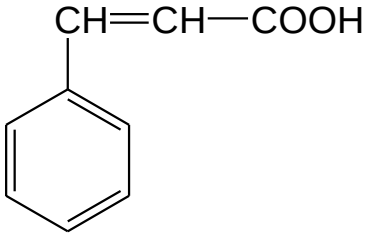
3-ciklohexil-propionsav



benzoesav



ftálsav



fahéjsav

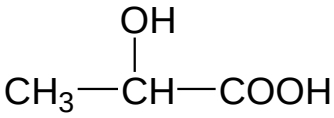
E) Láncban szubsztituált karbonsavak

$ClCH_2—COOH$

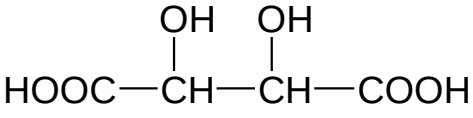
klórecetsav

$CF_3—COOH$

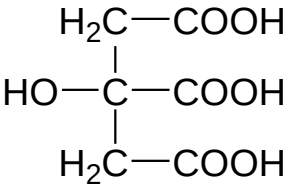
trifluorecetsav



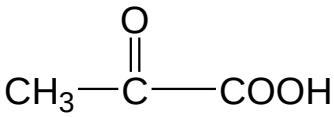
tejsav



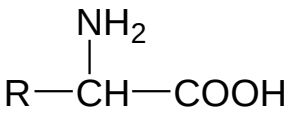
borkősav



citromsav

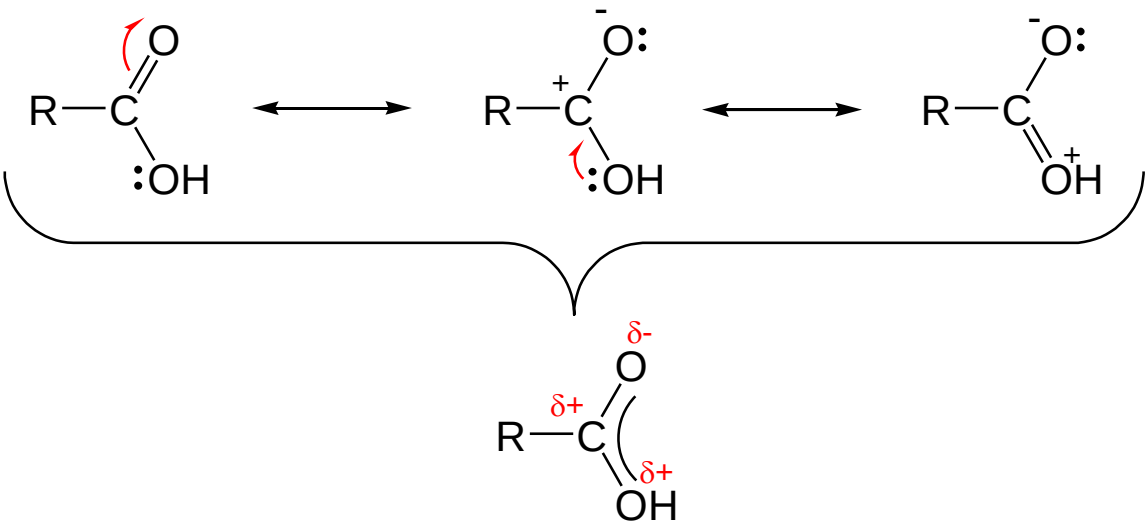


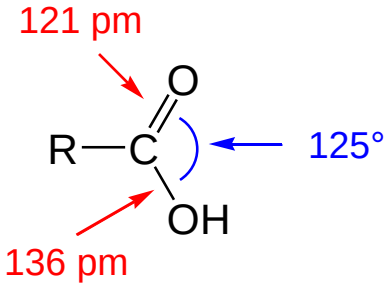
piroszőlősav

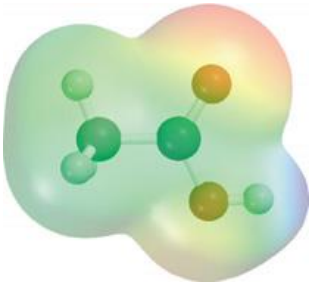


"α-aminosav"

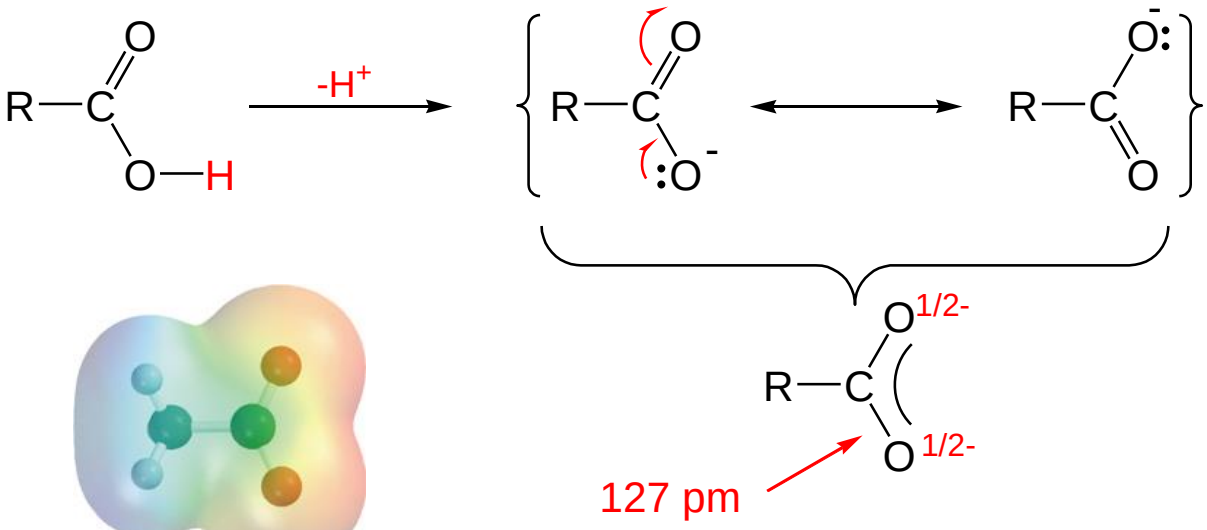
A karbonsavak szerkezete

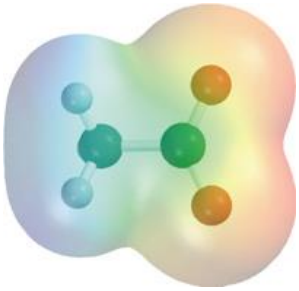






A karboxilátion szerkezete



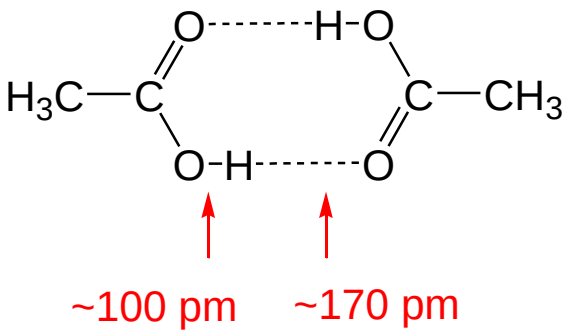


FIZIKAI TULAJDONSÁGOK

Forráspont

$CH_3—O—CH_3$	CH_3CH_2OH	CH_3COOH
-24 °C	78 °C	118 °C

Asszociáció hidrogénkötéssel (dimer szerkezet)



molekulatömeg x 2 = 120

fp: 118 °C

$CH_3(CH_2)_6CH_3$ (n-oktán)

molekulatömeg = 114

fp: 126 °C

$HOOC—COOH$	$CH_3COO—C_2H_5$
oxálsav	etil-acetát
op. = 190 °C	fp. = 77 °C

Vízoldhatóság

C_1-C_4: korlátlan; C_9-: oldhatatlan

Karbonsavak előállítása

Oxidációs reakciók

$$R{-}CH_2OH \longrightarrow R{-}CHO \longrightarrow R{-}COOH$$

(ld. alkoholok és oxovegyületek oxidációja)

$$R{-}CH{=}CR'R'' \longrightarrow R{-}COOH + R'R''CO$$

$$Ar{-}R \longrightarrow Ar{-}COOH$$

Karbonsavészterek- és nitrilek hidrolízise

(ld. karbonsavszármazékok hidrolízise)

$$\underset{\text{észter}}{R{-}COOR'} \longrightarrow R{-}COOH + R'{-}OH$$

$$\underset{\text{nitril}}{R{-}CN} \longrightarrow R{-}COOH$$

Grignard-reagens karboxilezése

$$\left[R{-}Br \xrightarrow{Mg} \right] R{-}MgBr \xrightarrow[2.\ H_3O^+]{1.\ CO_2} R{-}COOH$$

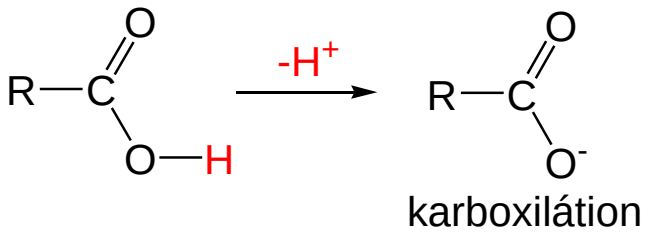
Malonészter-szintézis

(ld. karbonsavszármazékok)

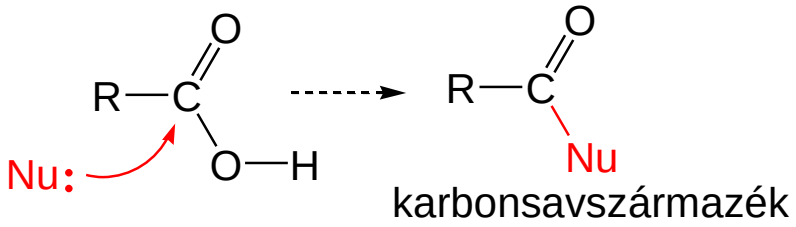
$$\underset{\text{malonészter}}{EtOOC{-}CH_2{-}COOEt} \xrightarrow{\text{4 lépés}} R{-}CH_2COOH$$

A karbonsavak reaktivitása (általános jellemzés)

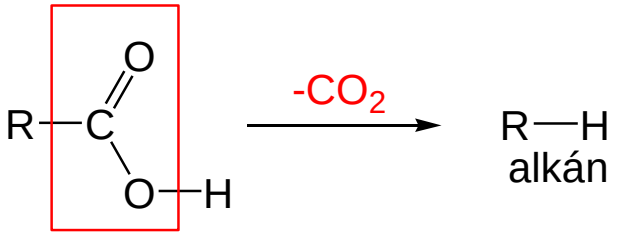
Savi jelleg



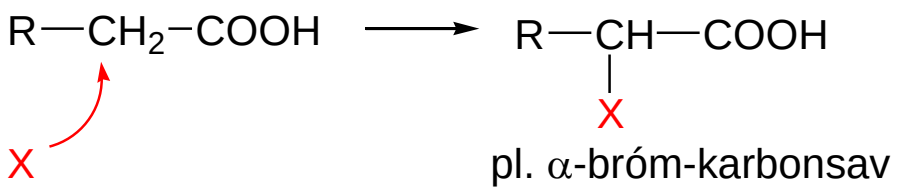
Szubsztitúció a karbonil-szénatomon



Dekarboxilezés



Szubsztitúció az α-szénatomon



A karbonsavak savi jellege

Etil-alkohol savassága

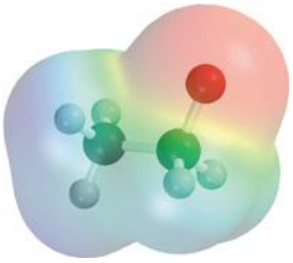
$$CH_3CH_2{-}O{-}H + H_2O \underset{}{\overset{\Delta G^0 = 91\ kJ/mol}{\rightleftharpoons}} CH_3CH_2{-}\ddot{O}^- + H_3O^+$$

etoxid-ion

$$K_s = \frac{[CH_3CH_2O^-][H_3O^+]}{[CH_3CH_2OH]} = 10^{-16} \qquad pK_s = 16{,}0$$

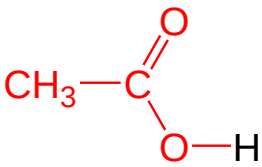
$CH_3CH_2{-}\ddot{O}^-$

etoxid-ion

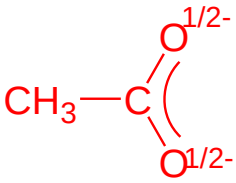


negatív töltés

Ecetsav savassága



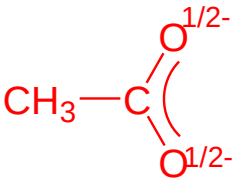
$$+ H_2O \underset{}{\overset{\Delta G^0 = 27\ kJ/mol}{\rightleftharpoons}}$$



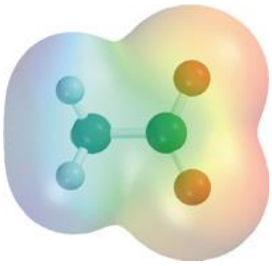
$$+ H_3O^+$$

acetát-ion

$$K_s = \frac{[CH_3COO^-][H_3O^+]}{[CH_3COOH]} = 1{,}8 \times 10^{-5} \qquad pK_s = 4.7$$



acetát-ion



negatív töltés

szimmetrikus elektronszerkezet

A karbonsavak sóképzési reakciói

Sav-bázis reakciók

víz $H_2O + H_2O \xrightleftharpoons{pk_s=15,7} OH^- + H_3O^+$

szénsav $H_2CO_3 + H_2O \xrightleftharpoons{pk_s=6,4} HCO_3^- + H_3O^+$

ecetsav $CH_3COOH + H_2O \xrightleftharpoons{pk_s=4,7} CH_3COO^- + H_3O^+$

H_2O H_2CO_3 CH_3COOH

savi erősség →

OH^- HCO_3^- CH_3COO^-

← bázis erősség

Sóképzés

$CH_3COOH + OH^- \longrightarrow CH_3COO^- + H_2O$

$CH_3COOH + HCO_3^- \longrightarrow CH_3COO^- + H_2CO_3\ (H_2O + CO_2)$

Tiszta karbonsav izolálása reakcióelegyből

nyerstermék (RCOOH + szerves és szervetlen szennyezések)

éter + víz

vizes fázis → vízoldható sók

szerves fázis → RCOOH + szerves szennyezések

+NaOH (H_2O)

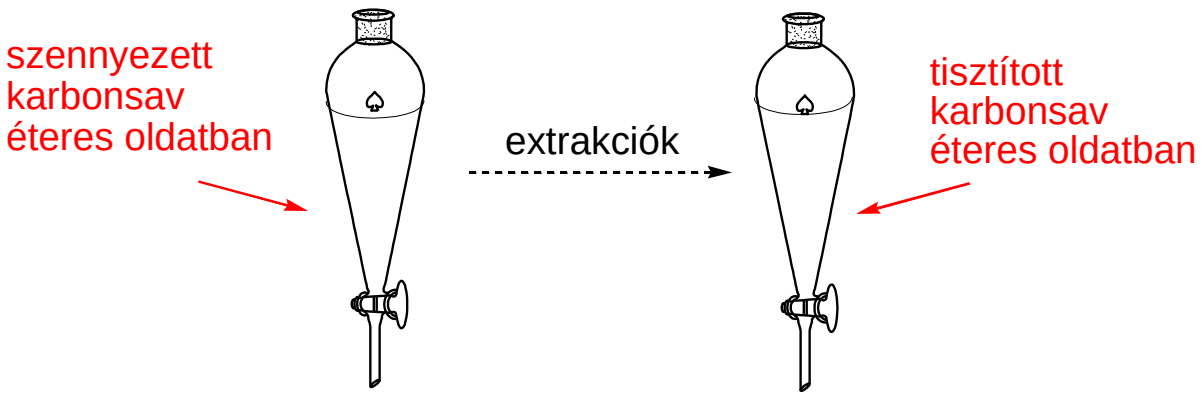
szerves fázis → szerves szennyezések

vizes fázis → RCOONa (H_2O)

+HCl + éter

vizes fázis → vízoldható sók

szerves fázis → RCOOH (éter)



Szubsztituált karbonsavak savi erőssége

$R \leftarrow COO^-$

-I effektusú R-csoport
növekvő stabilitású anion
erősebb sav

$R \rightarrow COO^-$

+I effektusú R-csoport
csökkenő stabilitású anion
gyengébb sav

Példák

	pK_s
$CH_3—COOH$ ecetsav	4.76
$Cl—CH_2—COOH$ klórecetsav	2.86
$Cl—CH(Cl)—COOH$ diklórecetsav	1.48
$Cl—C(Cl)_2—COOH$ triklórecetsav	0.70

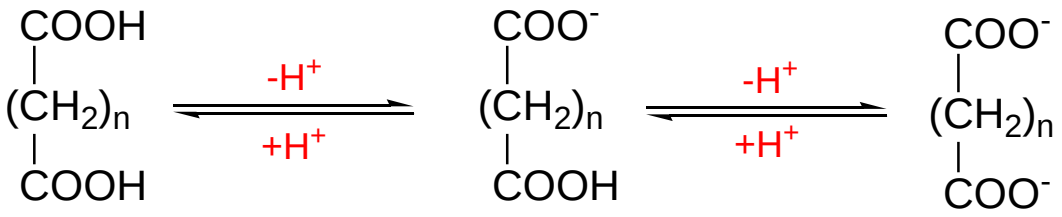
---

	pK_s
$CH_3CH_2CH_2COOH$ vajsav	4.82
$CH_2ClCH_2CH_2COOH$	4.50
$CH_3CHClCH_2COOH$	4.05
$CH_3CH_2CHClCOOH$	2.85

+I effektusú csoportok hatása

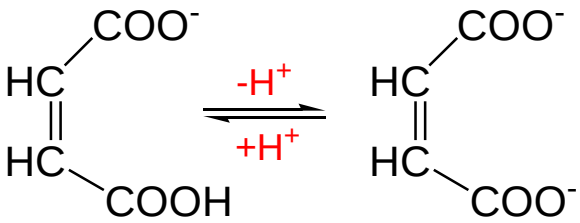
	pK_s
$H—COOH$	3.75
$CH_3—COOH$	4.76
$CH_3CH_2—COOH$	4.87
$(CH_3)_3C—COOH$	5.05

A dikarbonsavak savi jellege

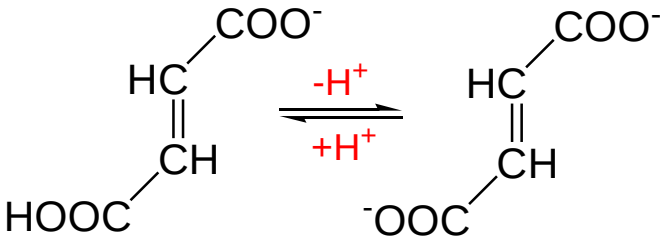


	n	pK_1	pK_2
oxálsav	0	1.27	4.28
malonsav	1	2.85	5.70
borostyánkősav	2	4.19	5.64

A térszerkezet hatása



maleinsav pK_{s2}=6.3



fumársav pK_{s2}=4.5

A KARBONSAVAK DEKARBOXILEZÉSE

$$R{-}COOH \xrightarrow{\text{hevítés}} R{-}H + CO_2$$

Példák

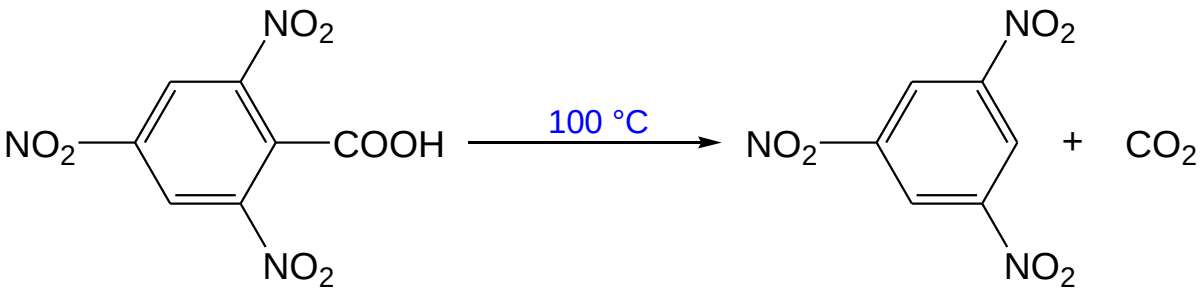
$$CH_3COONa + NaOH \xrightarrow[\text{(szilárd fázis)}]{\text{erős hevítés}} CH_4 + CO_2$$

nátrium-acetát

elektronvonzó csoport segít (pl. nitrocsoport)

$$NO_2{-}CH_2COOH \xrightarrow{150\ °C} NO_2CH_3 + CO_2$$

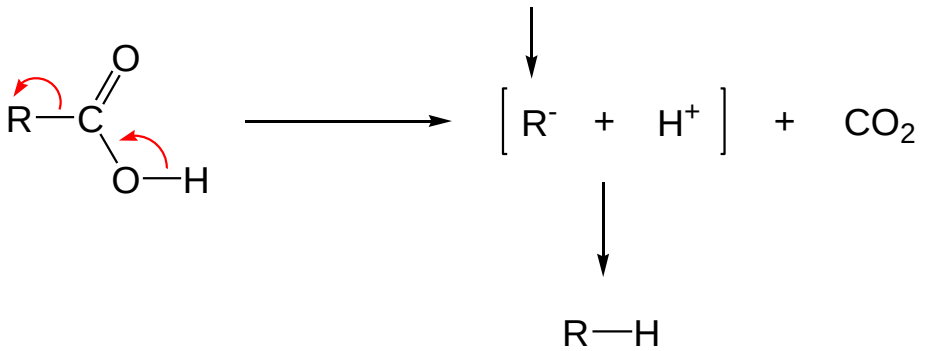
nitroecetsav



2,4,6-trinitrobenzoesav 2,4,6-trinitrobenzol

Mechanizmus

karbanion jellegű átmeneti állapot



A dikarbonsavak hevítése

dekarboxilezés

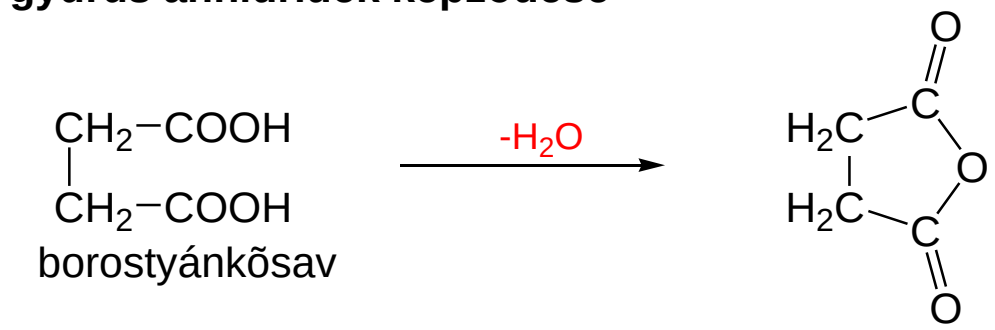
$$HOOC{-}COOH \longrightarrow HCOOH + CO_2$$

oxálsav

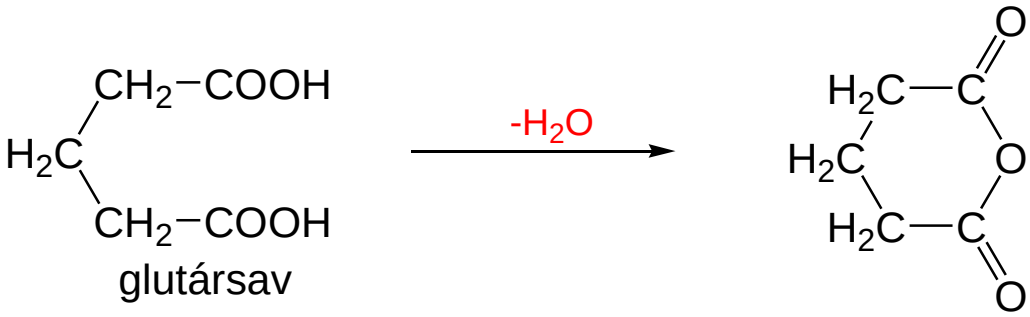
$$HOOC{-}CH_2{-}COOH \longrightarrow CH_3COOH + CO_2$$

malonsav

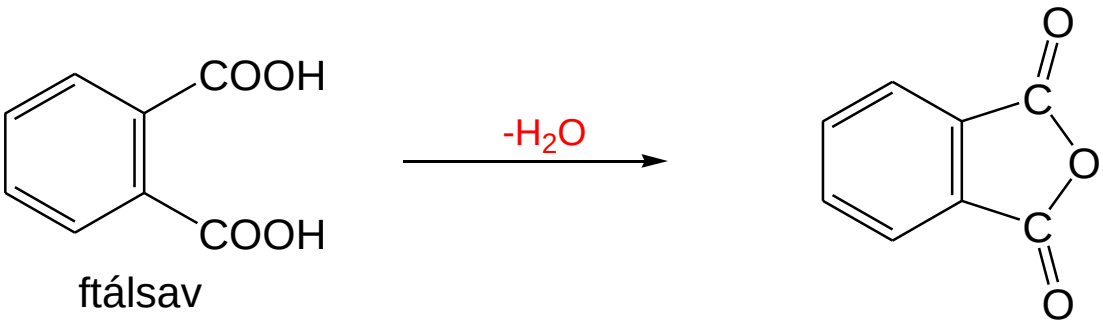
gyűrűs anhidridek képződése



borostyánkősav

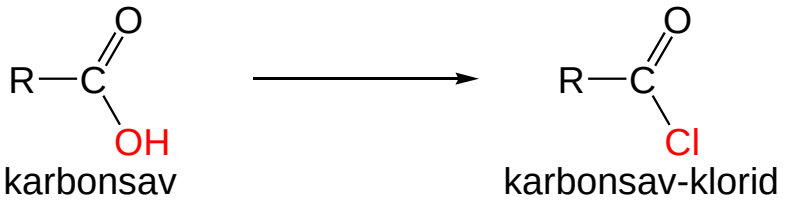


glutársav

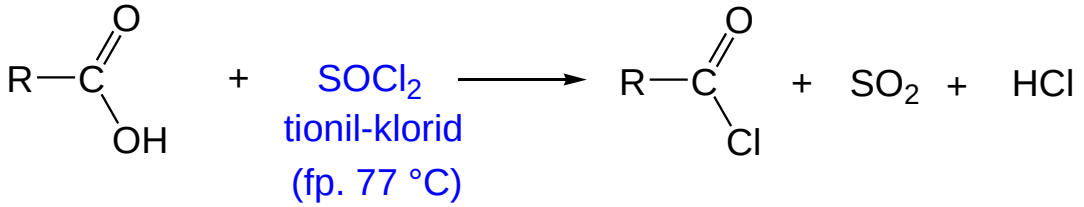


ftálsav

A KARBONSAVAK ÁTALAKÍTÁSA SAVKLORIDOKKÁ



A)



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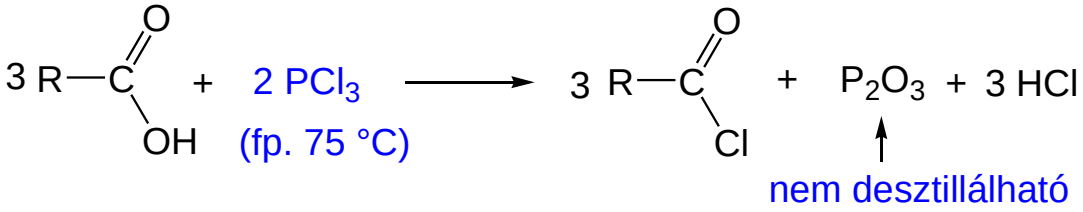

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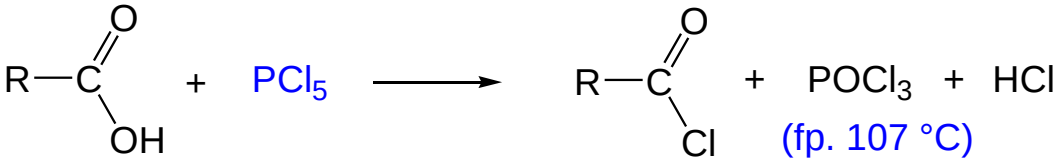
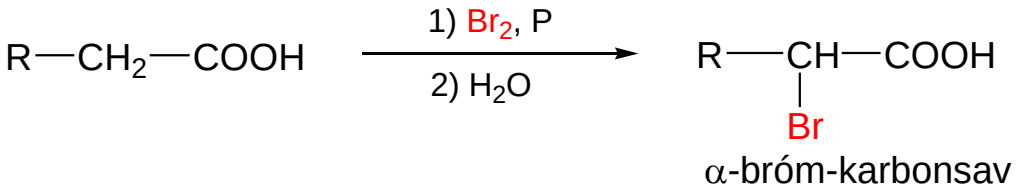
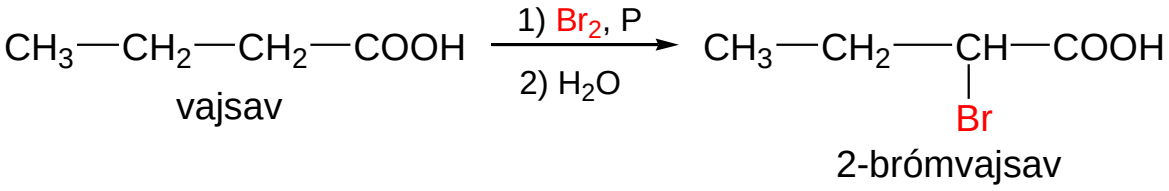


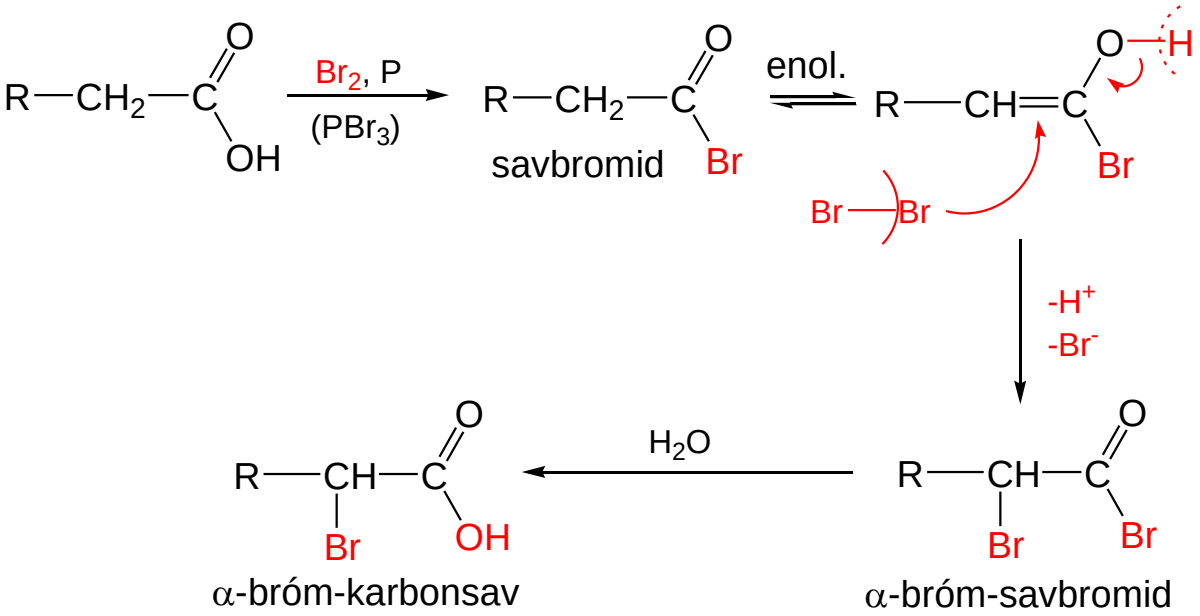
A KARBONSAVAK α-HELYZETŰ HALOGÉNEZÉSE



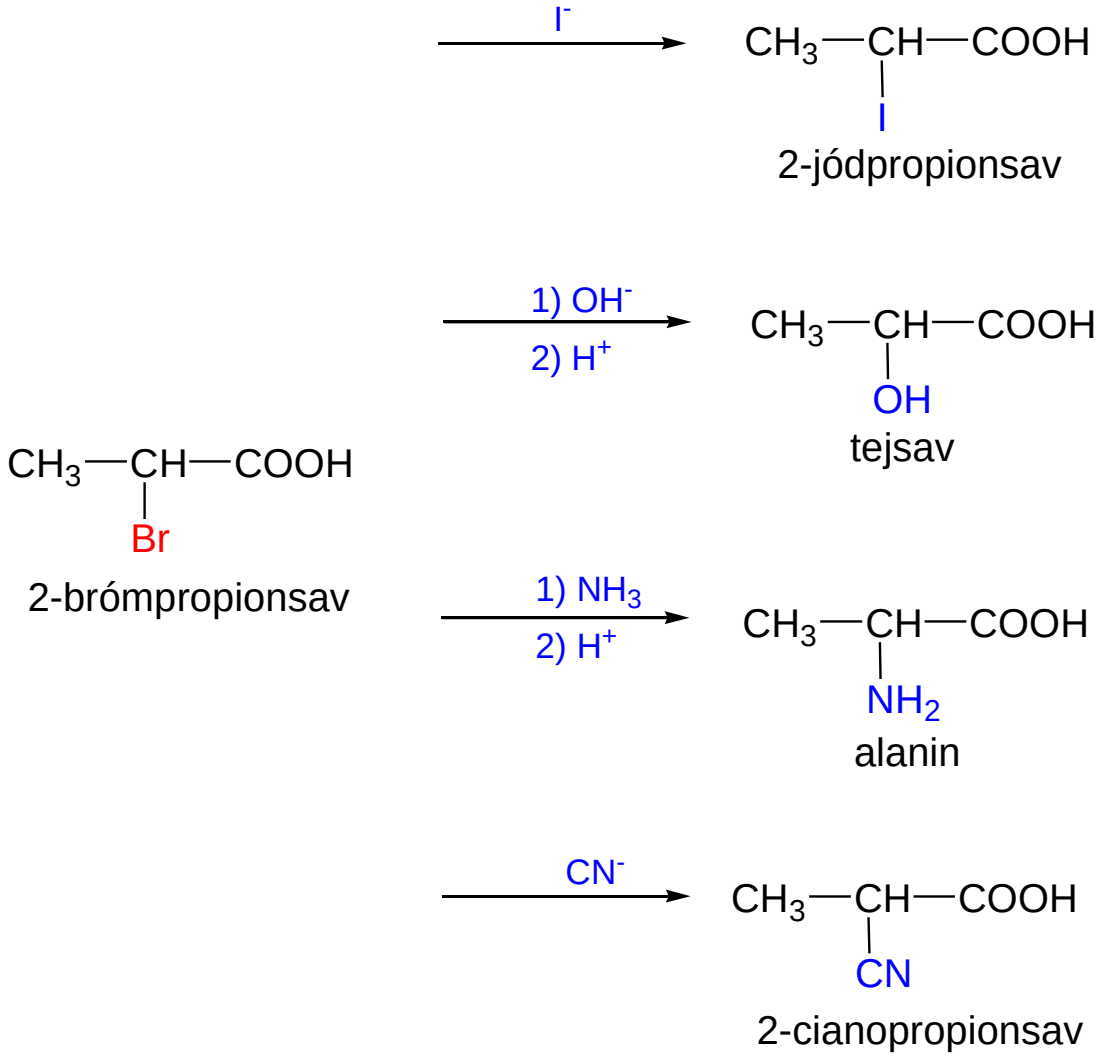
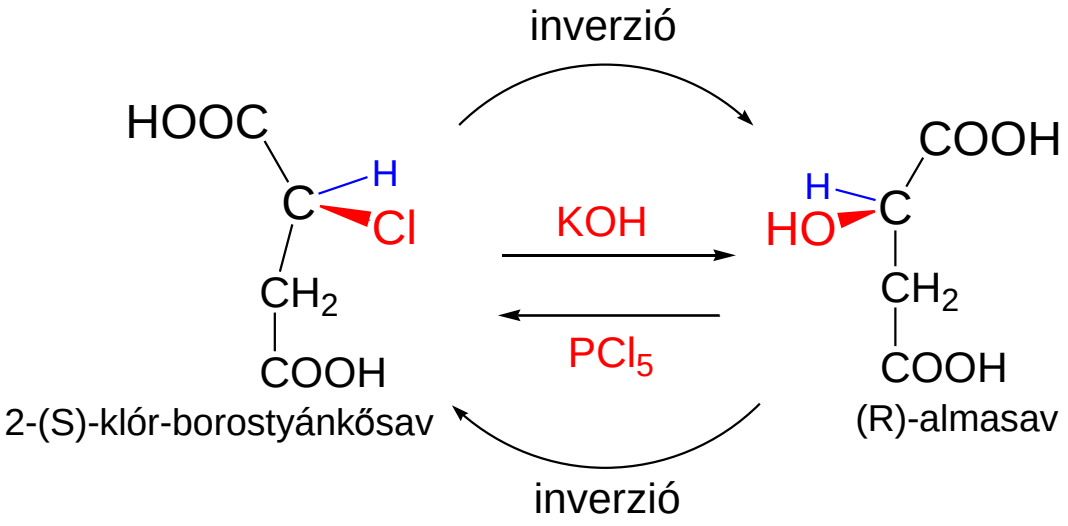
Példa



Mechanizmus



Az α-halogénezett karbonsavak reakciókészsége: S_N2 reakciók



Walden-inverzió, 1893 (S_N2 reakció inverziója)