## **ELECTRONIC SUPPLEMENTARY INFORMATION**

## Towards a greener synthesis of dianhydrohexitol esters

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Fig. S1 Dean-Stark apparatus for the esterification using Route 1



8,0E+08 7,0E+08 6,0E+08  $M = 146 \text{ g} \cdot \text{mol}^{-1}$ sd 5,0E+08 O/leug 0 3,0E+08 2,0E+08 1,0E+08 0,0E+00 25 50 100 125 150 175 75  $m/z /(g \cdot mol^{-1} \cdot C^{-1})$ 

Fig. S2 Mass spectra of isosorbide (left) and isomannide (right)



Fig. S3 Mass spectra of isomannide monoester 2-propionyl isomannide (left) and diester 2,5-dipropionyl isomannide (right); there were no further peaks beyond 175 and 225 gmol<sup>-1</sup> $C^{-1}$ 



Fig. S4 Mass spectra of isosorbide monoesters 2-propionyl isosorbide (left) and 5-propionyl isosorbide (right); there were no further peaks beyond 200 gmol<sup>-1</sup>C<sup>-1</sup>



Fig. S5 Mass spectra of isosorbide diester 2,5-dipropionyl isosorbide (left) and byproduct 5-propionyl-2-sulfon isosorbide (right); there were no further peaks beyond 200 gmol<sup>-1</sup>C<sup>-1</sup>



Fig. S6 <sup>1</sup>H NMR spectra of isosorbide (educt), 2,5-diacetyl isosorbide, 2,5-dipropionyl isosorbide and 2,5-dibutyryl isosorbide



Fig. S7 <sup>1</sup>H NMR spectra of isomannide, 2,5-diacetyl isomannide and 2,5-dipropionyl isomannide



Fig. S8 Reaction progress for the esterification of isosorbide with butyric acid: gas chromatograms of esterification of isosorbide with entrainer n-propyl acetate, mass spectra of the new peak 'a' at retention time 4.4 min indicating butyric acid propyl ester (right)



Fig. S9 Gas chromatograms of the purified dianhydrohexitol esters

## **OpenLCA data**

**Tab. S1** Elementary or process flows of chemicals and energy quantities for the production of 1000 kg DAIS; implemented processes are based on literature data; ecoinvent based product and elementary flows already contain the pre-processes from cradle-to-gate; output elementary flows are emissions which leave the product system under study and cause emissions and accordingly environmental impacts

Elementary or process flow	Quantity for the	Data source /Ecoinvent flows and processes used as
	production of 1t DAIS	assessment
Inputs Route 1	·	
Isosorbide	648.5kg	Implemented process based on literature data [1-4]
Glucose	1024.00 kg	Manufacture of starches and starch products: glucose production   glucose   Cutoff, U - GLO
Hydrogen, liquid	11.41 kg	Manufacture of basic chemicals: market for hydrogen, liquid   hydrogen, liquid   Cutoff, U - RER
Water, deionised	1530.61 kg	Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland
Energy for the catalytic hydrogenation of glucose to sorbitol	9776.26 kWh	Electric power generation, transmission and electricity voltage: transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - FR
Energy for the dehydration of sorbitol to isosorbide	6607.19 kWh	Electric power generation, transmission and electricity voltage: transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - FR
Energy and heat for the crystallisation of isosorbide	1027.36 kWh	Electric power generation, transmission and electricity voltage: transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - FR
Cooling water	40.53 m <sup>3</sup>	Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland
Acetic acid	1199.74 kg	Manufacture of basic chemicals: market for acetic acid, without water, in 98 % solution state   acetic acid, without water, in 98 % solution state   Cutoff, U - GLO
Amberlyst-15 (wet)	31.74 kg	Implemented process based on literature data [5]
Styrene	23.15 kg	Manufacture of plastics and synthetic rubber in primary forms: market for styrene   styrene   Cutoff, U - GLO
Divinylbenzene, produced from styrene and ethylene	3.50 kg	Implemented process based on literature data [6]
water, deionised	37.45 kg	Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland
Energy: polymerisation and functionalisation	122.51 kWh	Electric power generation, transmission and distribution: electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE
sulfuric acid	3.41 kg	Manufacture of basic precious and other non-ferrous metals: market for sulfuric acid   sulfuric acid   Cutoff, U - RER
carboxymethyl cellulose, powder	3.02 kg	Manufacture of basic chemicals: carboxymethyl cellulose production, powder   carboxymethyl cellulose, powder   Cutoff, U - RER
Entrainer: Toluene, liquid	Start: 2209.43 kg (recycle: 2099.50 kg)	Manufacture of basic chemicals: market for toluene, liquid   toluene, liquid   Cutoff, U – RER
n-propylacetate	Start: 2260.00 kg (recycle: 2147.00 kg)	Implemented process based on literature data [7]
Energy for chemicals production (pre-processes), for esterification [5], for DAIS purification [5]	20020.32 kWh 10573.58 kWh 3873.64 kWh	Electric power generation, transmission and distribution: electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE
Outputs Route 1		
Diacetyl isosorbide (DAIS)	1000.0 kg	set output
Acetic acid	62.8 kg	Elementary Flow: Emission to water/fresh water

Entrainer:       110.5 kg       Elementary Flow: Emission to water/fresh water         n-Propylacetate       113.0 kg       Elementary Flow: Emission to water/fresh water         Amberhyst.15 (wet and waste)       156.52 kg       Elementary Flow: Emission to water/fresh water         Polystyrene waste       31.74 kg       Elementary Flow: Emission to water/fresh water         Waste water from Amberlyst production, purification, functionalisation       2568.0 kg       Elementary Flow: Emission to water/fresh water         Waste water from isosorbid production from glucose       74940.0 kg       Elementary Flow: Emission to water/fresh water         Inputs Route 2       Isosorbide       634.78 kg       Implemented process based on literature data [1-4]         Acetic anhydride       804.8 kg       acetic anhydride production, ketene route   acetic anhydride   Cutoff, U - RER         Water for hydrolysis       10.5 kg       Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Lurope without         Energy for chemicals production (pre-processes), for DAS purification [5], for DAS purification [5]       31927.67 kWh         Outputs Route 2       bioactyl isosorbide       1000.0 kg         Diacetyl isosorbide       1000.0 kg       set upput         Acetic acid       1997.4 kg       implemented process based on literature data [1-4]         Acetic acid       1199.74 kg<			
Toluene       110.5 kg       Elementary Flow: Emission to water/fresh water         n-Propylacetate       113.0 kg       Elementary Flow: Emission to water/fresh water         Amberlyst-15 (wet and waste)       Elementary Flow: Emission to water/fresh water         Polystyrene waste       31.74 kg       Elementary Flow: Emission to water/fresh water         Production, purification, functionalisation       2568.0 kg       Elementary Flow: Emission to water/fresh water         Waste water from isosorbid       74940.0 kg       Elementary Flow: Emission to water/fresh water         production from glucose       Imputs Route 2       Isosorbide       634.78 kg         Isosorbide       634.78 kg       Implemented process based on literature data [1-4]         Acetic anhydride       804.8 kg       acetic anhydride production, ketene route   acetic anhydride processes), for sterification [5].         Water of hydrolysis       10.5 kg       Water collection, treatment and supply: market for water, deionised   vater, deionised   Cutoff, U - Europe without switzerland         Energy for chemicals production [5].       31927.67 kWh       electricity voltage transformation from high to medium voltage   cluoff, U - Europe without switzerland         Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route <td< td=""><td>Entrainer:</td><td></td><td></td></td<>	Entrainer:		
n-Propylacetate         113.0 kg         Elementary Flow: Emission to water/unspecified           Waste water (from esterification)         156.52 kg         Elementary Flow: Emission to water/fresh water           Amber/sst-15 (wet and waste)         31.74 kg         Elementary Flow: Emission to water/fresh water           Polystyrene waste         31.74 kg         Elementary Flow: Emission to water/fresh water           functionalisation         2568.0 kg         Elementary Flow: Emission to water/fresh water           Waste water from Sosorbid         74940.0 kg         Elementary Flow: Emission to water/fresh water           Inputs Rouce 2         Implemented process based on literature data [1-4]         actic anhydride production, ketner oroute   acetic (recycle 566.2 kg)           Acetic anhydride         804.8 kg         acetic anhydride   Cutoff, U - RER           Water for hydrolysis         10.5 kg         Water collection, treatment and supply: market for water, deionised   Autor, deionised   Cutoff, U - Europe without Switzerland           Energy for chemicals production (pre-processes), for orbals purification [5], 3960.66 kWh         of analyzer for acetic acid, without water, in 98% solution state   acetic acid           Outputs Reference Route         1000.0 kg         set output           Acetic acid         269.33 kg         Elementary Flow: Emission to water/fresh water           Inputs Reference Route         1199.74 kg         Implemented p	Toluene	110.5 kg	Elementary Flow: Emission to water/fresh water
Waste water (from esterification)       156.52 kg       Elementary Flow: Emission to water/fresh water         Amberlyst-15 (wet and waste)       31.74 kg       Elementary Flow: Waste/unspecified         Polystyrene waste       31.74 kg       Elementary Flow: Emission to water/fresh water         Waste water from Amberlyst       production, purification, purification, purification       2568.0 kg       Elementary Flow: Emission to water/fresh water         Waste water from isosorbid       74940.0 kg       Elementary Flow: Emission to water/fresh water         Inputs Route 2       isosorbide       634.78 kg       implemented process based on literature data [1-4]         Acetic anhydride       804.8 kg       acetic anhydride production, ketner route   acetic       (recycle 566.2 kg)         Water for hydrolysis       10.5 kg       Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland         Energy for chemicals production [5]       31927.67 kWh       electricity voltage transformation from high to medium voltage   electricity, medium voltage   cutoff, U - Europe without Switzerland         Tor esterification [5]       3960.66 kWh       collock kWh         for esterification [5]       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route       1199.74 kg       market for acetic acid, without water, in 98% solution state   acetic acid, without water, i	n-Propylacetate	113.0 kg	Elementary Flow: Emission to water/unspecified
Amberlyst-15 (wet and waste)         31.74 kg         Elementary Flow: Waste/unspecified           Polystyrene waste         31.74 kg         Elementary Flow: Waste/unspecified           Waste water from Amberlyst production, purification, functionalisation         2568.0 kg         Elementary Flow: Emission to water/fresh water           Waste water from isosorbid production from glucose         74940.0 kg         Elementary Flow: Emission to water/fresh water           Inputs Route 2         isosorbide         634.78 kg         Implemented process based on literature data [1-4]           Acetic anhydride         804.8 kg         acetic anhydride production, ketene route   acetic anhydride   Cutoff, U - RER           Water for hydrolysis         10.5 kg         Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland           Energy for chemicals production (pre-processes), for esterification [5], for ot suffication [5],         31927.67 kWh         electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE           Outputs Route 2         0000.06 kg         set output         Acetic acid         269.33 kg         Elementary Flow: Emission to water, fresh water           Inputs Reference Route         1199.74 kg         market for sufuric acid without water, in 98% solution state   acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% soluti	Waste water (from esterification)	156.52 kg	Elementary Flow: Emission to water/fresh water
Polystyrene waste       31.74 kg       Elementary Flow: Waste/unspecified         Waste water from Amberlyst production, purification, functionalisation       2568.0 kg       Elementary Flow: Emission to water/fresh water         Waste water from isosorbid       74940.0 kg       Elementary Flow: Emission to water/fresh water         Inputs Route 2       isosorbide       634.78 kg       acetic anhydride production, ketene route   acetic anhydride   Cutoff, U - RER         Vater for hydrolysis       10.5 kg       Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland         Energy for chemicals production (pre-processes), for esterification [5], 3960.66 kWh       31927.67 kWh       electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE         Outputs Route 2       1000.0 kg       set output         Acetic acid       269.33 kg       Elementary Flow: Emission to water, fresh water         Inputs Reference Route       1199.74 kg       market for suffuric acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLO <td>Amberlyst-15 (wet and waste)</td> <td></td> <td></td>	Amberlyst-15 (wet and waste)		
Waste water from Amberlyst production, purification, functionalisation       2568.0 kg       Elementary Flow: Emission to water/fresh water         Waste water from isosorbid production from glucose       74940.0 kg       Elementary Flow: Emission to water/fresh water         Inputs Route 2       isosorbide       634.78 kg       Implemented process based on literature data [1-4]         Acetic anhydride       804.8 kg       acetic anhydride production, ketene route   acetic anhydride production, reatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland         Energy for chemicals production (pre-processes), for esterification [5], dot esterification [5], dot pre-processes),       31927.67 kWh 1162.08 kWh       electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE         Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route       implemented process based on literature data [1-4]         Acetic acid       1199.74 kg       market for sodium bicarbonate   sodium bicarbonate   Cutoff, U - GLO         Sodium bicarbonate (NaHCO <sub>3</sub> )       950.29 kg       market for sulfuric acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLO      <	Polystyrene waste	31.74 kg	Elementary Flow: Waste/unspecified
production, purification, functionalisation       74940.0 kg       Elementary Flow: Emission to water/fresh water         Inputs Route 2       Implemented process based on literature data [1-4]         Acetic anhydride       634.78 kg       Implemented process based on literature data [1-4]         Acetic anhydride       804.8 kg       acetic anhydride production, ketene route   acetic         Water for hydrolysis       10.5 kg       Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without         Energy for chemicals production [5], for DAIS purification [5],       31927.67 kWh       electricity voltage transformation from high to medium voltage   electricity voltage transformation from high to medium voltage   Cutoff, U - DE         Outputs Route 2       Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route       Implemented process based on literature data [1-4]         Acetic acid       199.74 kg       market for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLO         Sodium bicarbonate (NaHCO <sub>3</sub> )       950.29 kg       market for sodium bicarbonate   Sodium bicarbonate   Sodium bicarbonate   Cutoff, U - BER         Toluene       2209.04 kg       Manufacture of basic chemicals: market for toluene, liquid   Cutoff, U - RER	Waste water from Amberlyst	2568.0 kg	Elementary Flow: Emission to water/fresh water
functionalisation         74940.0 kg           Waste water from isoorbid production from glucose         74940.0 kg           Inputs Route 2         Implemented process based on literature data [1-4]           Acetic anhydride         634.78 kg         acetic anhydride production, ketene route   acetic anhydride [Cutoff, U - RER           Water for hydrolysis         10.5 kg         Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland           Inputs Route 2         31927.67 kWh         voltage transformation from high to medium voltage   electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE           for DAIS purification [5].         3960.66 kWh         voltage transformation form high to medium voltage   electricity, medium voltage   Cutoff, U - DE           Diacetyl isosorbide         1000.0 kg         set output           Acetic acid         1199.74 kg         Implemented process based on literature data [1-4]           Acetic acid         1199.74 kg         market for sodium bicarbonate   sodium bicarbonate   Cutoff, U - GLO           Sodium bicarbonate (NaHCO <sub>3</sub> )         950.29 kg         market for sodium bicarbonate   sodium bicarbonate   Cutoff, U - GLO           Sulfuric acid         1.27 kg         market for sodium bicarbonate   cutoff, U - DE           Sodium bicarbonate (NaHCO <sub>3</sub> )         950.29 kg         Manufacture of basic chemical	production, purification,		
Waste water from isosorbid       74940.0 kg       Elementary Flow: Emission to water/fresh water         Inputs Route 2       isosorbide       634.78 kg       Implemented process based on literature data [1-4]         Acetic anhydride       804.8 kg       acetic anhydride production, ketene route   acetic anhydride   Cutoff, U - RER         Water for hydrolysis       10.5 kg       Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without Switzerland         Energy for chemicals production (pre-processes), for esterification [5], 3960.66 kWh       31927.67 kWh       electricity voltage transformation from high to medium voltage   Cutoff, U - DE         Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route       1199.74 kg       market for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLO         Sodium bicarbonate (NaHCO3)       950.29 kg       market for sulfuric acid   sulfuric acid   Cutoff, U - RER         Toluene       2209.04 kg       Manufacture of basic chemicals: market for toluene, liquid   toluen	functionalisation		
production from glucose         Implemented process based on literature data [1-4]           Isosorbide         634.78 kg         Implemented process based on literature data [1-4]           Acetic anhydride         804.8 kg         acetic anhydride production, ketene route   acetic           Water for hydrolysis         10.5 kg         Water collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without           Switzerland         Switzerland         Switzerland           Energy for chemicals production [5], does been for esterification [5], does been for acetic acid, without water, in 98% solution state   acetic acid           Inputs Reference Route         1000.0 kg         set output           Isosorbide         634.78 kg         Implemented process based on literature data [1-4]           Acetic acid         269.33 kg         Elementary Flow: Emission to water/fresh water           Inputs Reference Route         Implemented process based on literature data [1-4]           Acetic acid         1199.74 kg         market for sodium bicarbonate   sodium bicarbonate   Cutoff, U - GLO           Sodium bicarbonate (NaHCO3)         950.29 kg         market for solium caid   sulfuric acid   cutoff, U - RER           Toluene         2209.04 kg	Waste water from isosorbid	74940.0 kg	Elementary Flow: Emission to water/fresh water
Inputs Route 2Isosorbide634.78 kgImplemented process based on literature data [1-4]Acetic anhydride804.8 kgacetic anhydride production, ketene route   aceticWater for hydrolysis10.5 kgWater collection, treatment and supply: market for water, deionised   water, deionised   water, deio	production from glucose		
Isosorbide634.78 kgImplemented process based on literature data [1-4]Acetic anhydride804.8 kg (recycle 566.2 kg)acetic anhydride production, ketene route   acetic anhydride   Cutoff, U - RERWater for hydrolysis10.5 kgWater collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without SwitzerlandEnergy for chemicals production (pre-processes), for esterification [5], for DAIS purification [5]31927.67 kWh 1162.08 kWh 3960.66 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEOutputs Route 2 Diacetyl isosorbide1000.0 kgset output Acetic acid269.33 kgInputs Reference Route Tosorbide1000.0 kgset output state   acetic acid, without water, in 98% solution state   acetic acid   Sulfuric acid   Cutoff, U - RERToluene2209.04 kg (recycle 2099.5 kg)Manufacture of basic chemicals: market for toluene, liquid [ toluene, liquid   Cutoff, U - BEREnergy for chemicals production (pre-processes), for esterification [5], 387.22 kWh28479.14 kWh set outputDiacetyl isosorbide1000.0 kgset output Cutoff, U - BERAcetic acid678.0 kgElementary Flow: Emission to water/fresh waterToluene100.0 kgset output Set outputAcetic acid678.0 kgElementary Flo	Inputs Route 2		1
Acetic anhydride804.8 kg (recycle 566.2 kg)acetic anhydride production, ketene route   acetic anhydride   Cutoff, U - RERWater for hydrolysis10.5 kgWater collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without SwitzerlandEnergy for chemicals production (pre-processes), for esterification [5], Biacetyl isosorbide31927.67 kWh 162.08 kWh 3960.66 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEOutputs Route 2 Diacetyl isosorbide1000.0 kg 269.33 kgElementary Flow: Emission to water/fresh waterInputs Reference Route Isosorbide1199.74 kgmarket for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLOSodium bicarbonate (NaHCO3)950.29 kgmarket for solfum bicarbonate   sodium bicarbonate   Cutoff, U - GLOSulfuric acid1.27 kgmarket for solfum bicarbonate   sodium bicarbonate   (recycle 2099.5 kg)Energy for chemicals production (pre-processes), for actir acid28479.14 kWh 9163.77 kWhOutputs Reference Route28479.14 kWh 9163.77 kWhelectricity, medium voltage   Cutoff, U - DEDiacetyl isosorbide1000.0 kgset outputCutoff, U - GLO28479.14 kWh 9163.77 kWhfor electricity, medium voltage   Cutoff, U - DEDiacetyl isosorbide1000.0 kgset outputCutoff, U - DE9163.77 kWhelectricity, medium voltage   Cutoff, U - DEOutputs Reference Route1000.0 kgset outputDiacetyl isosor	Isosorbide	634.78 kg	Implemented process based on literature data [1-4]
Image: constraint of the second sec	Acetic anhydride	804.8 kg	acetic anhydride production, ketene route   acetic
Water for hydrolysis10.5 kgWater collection, treatment and supply: market for water, deionised   water, deionised   Cutoff, U - Europe without SwitzerlandEnergy for chemicals production (pre-processes), for esterification [5], of DAIS purification [5]31927.67 kWh 1162.08 kWh 3960.66 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEOutputs Route 23960.66 kWhvoltage   electricity, medium voltage   Cutoff, U - DEDiacetyl isosorbide1000.0 kgset outputAcetic acid269.33 kgElementary Flow: Emission to water/fresh waterInputs Reference Route1199.74 kgmarket for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLOSodium bicarbonate (NaHCO3)950.29 kgmarket for sulfuric acid   Cutoff, U - DEFor exertification [5]3874.22 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEOutputs Reference Route1000.0 kgset outputCatic acid678.0 kgElementary Flow: Emission to water/fresh waterToluene110.5 kgElementary Flow: Emission to water/fresh waterMarcaric acid isosorbide1000.0 kgset output <td></td> <td>(recycle 566.2 kg)</td> <td>anhydride   Cutoff, U - RER</td>		(recycle 566.2 kg)	anhydride   Cutoff, U - RER
deionised   water, deionised   Cutoff, U - Europe without SwitzerlandEnergy for chemicals production (pre-processes), for esterification [5], B0ALS purification [5]31927.67 kWh 1162.08 kWh 3960.66 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEOutputs Route 2Diacetyl isosorbide1000.0 kgset outputAcetic acid269.33 kgElementary Flow: Emission to water/fresh waterInputs Reference Route1199.74 kgmarket for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLOSodium bicarbonate (NaHCO3)950.29 kgmarket for solum bicarbonate   sodium bicarbonate   Cutoff, U - GLOSulfuric acid1.27 kgmarket for sulfuric acid   sulfuric acid   Cutoff, U - RERToluene2209.04 kg (recycle 2099.5 kg)Manufacture of basic chemicals: market for toluene, liquid toluene, liquid   Cutoff, U - REREnergy for chemicals production (pre-processes), for acetrification [5], 	Water for hydrolysis	10.5 kg	Water collection, treatment and supply: market for water,
SwitzerlandEnergy for chemicals production (pre-processes), for esterification [5], for DAIS purification [5]31927.67 kWh 1162.08 kWh 3960.66 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEOutputs Route 2Diacetyl isosorbide1000.0 kgset outputAcetic acid269.33 kgElementary Flow: Emission to water/fresh waterInputs Reference RouteIsosorbide634.78 kgImplemented process based on literature data [1-4]Acetic acid1199.74 kgmarket for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLOSodium bicarbonate (NaHCO3)950.29 kgmarket for solium bicarbonate   sodium bicarbonate   Cutoff, U - GLOSulfuric acid1.27 kgmarket for sulfuric acid   sulfuric acid   Cutoff, U - RERToluene2209.04 kg (recycle 2099.5 kg)Manufacture of basic chemicals: market for toluene, liquid (toluene, liquid   Cutoff, U - NEREnergy for chemicals production (pre-processes), for esterification [5], 9163.77 kWh28479.14 kWh 9163.77 kWhMoutgae   electricity, medium voltage   Cutoff, U - DE28479.14 kWh voltage   electricity, medium voltage   Cutoff, U - DEDiacetyl isosorbide1000.0 kgset outputAcetic acid678.0 kgElementary Flow: Emission to water/fresh waterDiacetyl isosorbide1000.0 kgset outputAcetic acid678.0 kgElementary Flow: Emission to water/fresh waterDutputs Reference Route110.5			deionised   water, deionised   Cutoff, U - Europe without
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for esterification [5], for DAIS purification [5]       3960.66 kWh         Outputs Route 2         Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route       isosorbide       634.78 kg       Implemented process based on literature data [1-4]         Acetic acid       1199.74 kg       market for acetic acid, without water, in 98% solution state   acetic acid, without water, in 98% solution state   Cutoff, U - GLO         Sodium bicarbonate (NaHCO <sub>3</sub> )       950.29 kg       market for solium bicarbonate   sodium bicarbonate   cutoff, U - GLO         Sulfuric acid       1.27 kg       market for sulfuric acid   sulfuric acid   Cutoff, U - RER         Toluene       2209.04 kg       Manufacture of basic chemicals: market for toluene, liquid (recycle 2099.5 kg)         If or esterification [5], 9163.77 kWh       voltage   electricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DE         Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       678.0 kg       Elementary Flow: Emission to water/fresh water         Toluene       1105.5 kg       Elementary Flow: Emission to water/fresh water         Diacetyl isosorbide       1000.0 kg       set output         Acetic acid       678.0 kg       Elementary Flow	(pre-processes),	1162.08 kWh	voltage   electricity, medium voltage   Cutoff, U - DE
for DAIS purification [5]       Image: Set output         Outputs Route 2       1000.0 kg       set output         Diacetyl isosorbide       269.33 kg       Elementary Flow: Emission to water/fresh water         Inputs Reference Route       Isosorbide       634.78 kg       Implemented process based on literature data [1-4]         Acetic acid       1199.74 kg       market for acetic acid, without water, in 98% solution state   cutoff, U - GLO         Sodium bicarbonate (NaHCO <sub>3</sub> )       950.29 kg       market for sodium bicarbonate   sodium bicarbonate   cutoff, U - GLO         Sulfuric acid       1.27 kg       market for sulfuric acid   sulfuric acid   Cutoff, U - RER         Toluene       2209.04 kg       Manufacture of basic chemicals: market for toluene, liquid   recycle 2099.5 kg)         toluene, liquid   Cutoff, U - RER         Energy for chemicals production (pre-processes), for esterification [5], 9163.77 kWh       943.77 kWh       voltage   electricity, medium voltage   Cutoff, U - DE         Diacetyl isosorbide       1000.0 kg       set output       Acetic acid       678.0 kg       Elementary Flow: Emission to water/fresh water         Toluene       110.5 kg       Elementary Flow: Emission to water/fresh water       Toluene flow: Emission to water/fresh water	for esterification [5],	3960.66 kWh	
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Cutoff, U - GLOSodium bicarbonate (NaHCO3)950.29 kgmarket for sodium bicarbonate   sodium bicarbonate   Cutoff, U - GLOSulfuric acid1.27 kgmarket for sulfuric acid   sulfuric acid   Cutoff, U - RERToluene2209.04 kg (recycle 2099.5 kg)Manufacture of basic chemicals: market for toluene, liquid   toluene, liquid   Cutoff, U - REREnergy for chemicals production (pre-processes), for esterification [5], or DAIS purification [5]28479.14 kWh 9163.77 kWh 3874.22 kWhelectricity voltage transformation from high to medium voltage   electricity, medium voltage   Cutoff, U - DEDiacetyl isosorbide1000.0 kgset outputAcetic acid678.0 kgElementary Flow: Emission to water/fresh waterToluene110.5 kgElementary Flow: Emission to water/fresh waterWaste water (containing neutralized sulfuric acid)11456.5 kgElementary Flow: Emission to water/fresh water			state   acetic acid, without water, in 98% solution state
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for DAIS purification [5]       3874.22 kWh         Outputs Reference Route         Diacetyl isosorbide       1000.0 kg         Acetic acid       678.0 kg         Elementary Flow: Emission to water/fresh water         Toluene       110.5 kg         Waste water (containing neutralized sulfuric acid)       11456.5 kg         Elementary Flow: Emission to water/fresh water	for esterification [5],	9163.77 kWh	
Outputs Reference Route           Diacetyl isosorbide         1000.0 kg         set output           Acetic acid         678.0 kg         Elementary Flow: Emission to water/fresh water           Toluene         110.5 kg         Elementary Flow: Emission to water/fresh water           Waste water (containing neutralized sulfuric acid)         11456.5 kg         Elementary Flow: Emission to water/fresh water	for DAIS purification [5]	3874.22 kWh	
Diacetyl isosorbide         1000.0 kg         set output           Acetic acid         678.0 kg         Elementary Flow: Emission to water/fresh water           Toluene         110.5 kg         Elementary Flow: Emission to water/fresh water           Waste water (containing neutralized sulfuric acid)         11456.5 kg         Elementary Flow: Emission to water/fresh water	Outputs Reference Route		·
Acetic acid     678.0 kg     Elementary Flow: Emission to water/fresh water       Toluene     110.5 kg     Elementary Flow: Emission to water/fresh water       Waste water (containing neutralized sulfuric acid)     11456.5 kg     Elementary Flow: Emission to water/fresh water	Diacetyl isosorbide	1000.0 kg	set output
Toluene     110.5 kg     Elementary Flow: Emission to water/fresh water       Waste water (containing neutralized sulfuric acid)     11456.5 kg     Elementary Flow: Emission to water/fresh water	Acetic acid	678.0 kg	Elementary Flow: Emission to water/fresh water
Waste water (containing neutralized sulfuric acid)     11456.5 kg     Elementary Flow: Emission to water/fresh water	Toluene	110.5 kg	Elementary Flow: Emission to water/fresh water
neutralized sulfuric acid)	Waste water (containing	11456.5 kg	Elementary Flow: Emission to water/fresh water
	neutralized sulfuric acid)		
Sodium sulfate 1.27 kg   Elementary Flow: Resource/unspecified	Cadium culfata	1.27 kg	Elementary Elow: Resource/unspecified

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