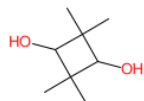




TOX ERASER FCM - REPORT

ANALYSIS RESULTS FOR TARGET MOLECULE: OC1C(C)(C)C(O)C1(C)(C)

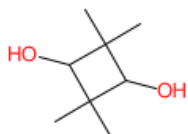
TOX ERASER FCM VERSION - 0.8.1



Target Compound:
OC1C(C)(C)C(O)C1(C)(C)

Molecule was found in ANNEX I list
Molecule was not found in SCIL list

Matched molecule from ANNEX I list



Similarity Index: 1

Molecule Name: 2,2,4,4-tetramethylcyclobutane-1,3-diol (TMCD)

CAS: 3010-96-6

Vega SMILES: OC1C(C)(C)C(O)C1(C)(C)

[EU Commission Regulation 10/2011]

Ref Number: 25187

FCM Number: 881

Use as additive or polymer production aid (yes/no): no

Use as monomer or other starting substance or macromolecule obtained from microbial fermentation (yes/no): yes

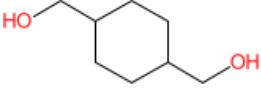
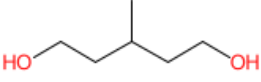

FRF applicable (yes/no): no

SML [mg/kg]: 5

Restrictions and specifications: Only for: (a) repeated use articles for long term storage at room temperature or below and hotfill; (b) single use materials and articles as a co-monomer at a maximum use level of 35 mole % of the diol component of polyesters, and if such materials and articles are for long term storage at room temperature or below of food types which have an alcohol content of up to 10 % and for which Table 2 of Annex III does not assign simulant D2. Hot fill conditions are allowed for such single use materials and articles.

Amendment : 2015/174

5 other compounds found in ANNEX I list

	<p>Similarity Index: 0,88</p> <p>Molecule Name: 1,4-Bis(hydroxymethyl)cyclohexane</p> <p>CAS: 08/07/05</p> <p>Vega SMILES: OCC1CCC(CO)CC1</p> <p>[EU Commission Regulation 10/2011] Ref Number: 13390, 14880 FCM Number: 210 Use as additive or polymer production aid (yes/no): no Use as monomer or other starting substance or macromolecule obtained from microbial fermentation (yes/no): yes FRF applicable (yes/no): no</p>
	<p>Similarity Index: 0,88</p> <p>Molecule Name: 3-Methyl-1,5-pentanediol</p> <p>CAS: 4457-71-0</p> <p>Vega SMILES: OCCC(C)CCO</p> <p>[EU Commission Regulation 10/2011] Ref Number: 22074 FCM Number: 883 Use as additive or polymer production aid (yes/no): no Use as monomer or other starting substance or macromolecule obtained from microbial fermentation (yes/no): yes FRF applicable (yes/no): no SML [mg/kg]: 0,05 Restrictions and specifications: Only to be used in materials in contact with food at a surface to mass ratio up to 0.5 dm²/kg</p>
	<p>Similarity Index: 0,86</p> <p>Molecule Name: 1,1,1-Trimethylolpropane</p> <p>CAS: 77-99-6</p> <p>Vega SMILES: OCC(CO)(CO)CC</p> <p>[EU Commission Regulation 10/2011] Ref Number: 13380, 25600, 39560, 94960 FCM Number: 141 Use as additive or polymer production aid (yes/no): yes Use as monomer or other starting substance or macromolecule obtained from microbial fermentation (yes/no): yes FRF applicable (yes/no): no SML [mg/kg]: 6</p>

Similarity Index: 0,86

Molecule Name: 1,6-Hexanediol

CAS: 11/08/29



Vega SMILES: OCCCCCCO

[EU Commission Regulation 10/2011]

Ref Number: 18700

FCM Number: 361

Use as additive or polymer production aid (yes/no): no

Use as monomer or other starting substance or macromolecule obtained from microbial fermentation (yes/no): yes

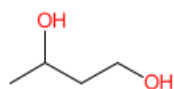
FRF applicable (yes/no): no

SML [mg/kg]: 0,05

Similarity Index: 0,85

Molecule Name: 1,3-Butanediol

CAS: 107-88-0



Vega SMILES: OCC(O)C

[EU Commission Regulation 10/2011]

Ref Number: 13690

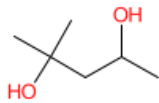
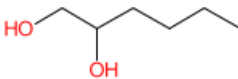
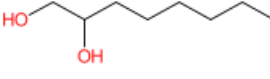
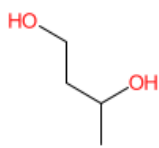
FCM Number: 228

Use as additive or polymer production aid (yes/no): no

Use as monomer or other starting substance or macromolecule obtained from microbial fermentation (yes/no): yes

FRF applicable (yes/no): no

5 other compounds found in SCIL list

	<p>Similarity Index: 0,9</p> <p>Molecule Name: 2-Methyl-2,4-pentanediol</p> <p>CAS: 107-41-5</p> <p>Vega SMILES: <chem>OC(C)CC(O)(C)C</chem></p> <p>Included in SCIL list (low concern based on experimental and modelled data): yes</p>
	<p>Similarity Index: 0,87</p> <p>Molecule Name: pentyleneglycol</p> <p>CAS: 5343-92-0</p> <p>Vega SMILES: <chem>OCC(O)CCC</chem></p> <p>Included in SCIL list (low concern based on experimental and modelled data): yes</p>
	<p>Similarity Index: 0,87</p> <p>Molecule Name: 1,2-Hexanediol</p> <p>CAS: 6920-22-5</p> <p>Vega SMILES: <chem>OCC(O)CCCC</chem></p> <p>Included in SCIL list (low concern based on experimental and modelled data): yes</p>
	<p>Similarity Index: 0,86</p> <p>Molecule Name: Caprylyl glycol</p> <p>CAS: 1117-86-8</p> <p>Vega SMILES: <chem>OCC(O)CCCCCC</chem></p> <p>Included in SCIL list (low concern based on experimental and modelled data): yes</p>
	<p>Similarity Index: 0,85</p> <p>Molecule Name: 1,3-Butanediol</p> <p>CAS: 107-88-0</p> <p>Vega SMILES: <chem>OCCC(O)C</chem></p> <p>Included in SCIL list (low concern based on experimental and modelled data): yes</p>