



Version	SUBSTANCE IDENTIFICATION PROFILE (SIP)
v.4	
21/06/2023	

No	1.1. Chemical Name	1.2. EC Number	1.3. CAS Number	1.4. Composition Type
IP24	Pentacalcium hydroxide tris(orthophosphate)	235-330-6	12167-74-7	mono-constituent substance

This Substance Identification Profile (SIP) is developed to represent the Identification parameters of the substance described in line with the Substance Identification requirements of REACH Annex VI and relevant guidance for the purpose of identifying the registered substance and the provision of a 'boundary composition' for IUCLID 6 dossier updates.

Reference	SI Parameter	Value / Not necessary / Not for SIP	Remark / Justification
2.1.A	Name or other Identifiers of the substance		
	CAS (hydrates)	1306-06-5, 12167-74-7, 68439-86-1	
	Synonyms	Hydroxylapatite / Hydroxy Apatite, Calcium Hydroxide Phosphate, Pentacalcium Hydroxy Monophosphate, Tricalcium Phosphate (frequently used commercial name), Bone ash	
	SMILES	[OH-].[O-]P(=O)([O-])[O-].[O-]P(=O)([O-])[O-].[O-]P(=O)([O-])[O-].[Ca+2].[Ca+2].[Ca+2].[Ca+2]	
	Molecular formula	Ca ₅ (PO ₄) ₃ OH or 10 CaO ₃ (P ₂ O ₅)H ₂ O or Ca ₅ HO ₁₃ P ₃	
	Structural image / diagram (indicative)		
	EU food legislation number / INS n°	E341iii	same as IP23
	State / form	Solid: Particulate / Powder	
	Granulometry range	Up to 100% of particles have a diameter of <100µm.	The registration dossier will take into account the inhalation risk. Nanoforms of the substance have been identified and testing is ongoing, the dossier and SIP will be



			updated when the testing is concluded (expected for mid 2024).
	pH range for aqueous solutions	pH of solution in water solubility test was pH 7.2 - 7.4. pH of 10 % suspension acc. to DIN EN ISO 797-9: 7.5 - 10.5	
2.1.B	Substances (with core identifiers) also falling under this substance (with justification)		
	Name or other Identifiers of the substance	Hydroxylapatite, Bone ash	
	EC Number	215-145-7, 270-423-5	
	CAS number	1306-06-5, 68439-86-1	
	Additional information		
2.3	Chemical Composition of the substance		
2.3.1	Main Constituent		
	Name	Pentacalcium hydroxide tris(orthophosphate)	
	Typical concentration (%w/w)	80%	
	Concentration range (%w/w)	>70 -100%	
2.3.2	Typical Impurity / Impurities (above 1% or lower if contributing to the hazard or PBT profile) - create repeat blocks if necessary		
2.3.2.1	Name -Impurity (1)	Calcium hydrogenorthophosphate	
	CAS Number -Impurity (1)	7757-93-9	
	EC Number -Impurity (1)	231-826-1	
	Molecular Formula - Impurity (1)	CaHPO4	
	Typical concentration (%w/w) -Impurity (1)	ca. 3%	
	Concentration range (%w/w) -Impurity (1)	0 - 20%	
	Relevant for classification and labelling?	N	
2.3.3	Additives - create block similar to impurities if relevant		
	Not relevant		
2.4	Classification and labelling		
	Not classified		
2.5	Justification for deviation from substance identity rules		
<p>In accordance with ECHA Guidance for identification and naming of substances under REACH and CLP, version 1.4, when the concentration of the main constituent is <70% the following requirement(s) are met:</p> <p>1. The substance has been shown to have similar physico-chemical properties and the same hazard profile as other mono-constituent substances with the same identity that fulfil the 80% rule. and/or</p> <p>2. The range of concentrations for the main constituent and the impurities overlap the 80% criterion and the main constituent is only occasionally ≤ 80%.</p>			