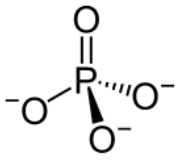


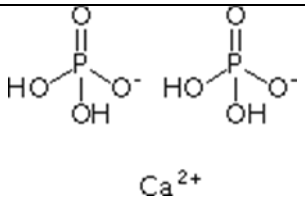
Inorganic Phosphates REACH Consortium

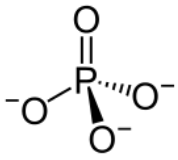
Version
v.5
13/06/2023

SUBSTANCE IDENTIFICATION PROFILE (SIP)

No	1.1. Chemical Name	1.2. EC Number	1.3. CAS Number	1.4. Composition Type
IP21	Calcium bis(dihydrogen-orthophosphate)	231-837-1	7758-23-8	mono-constituent

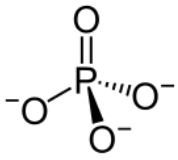
This Substance Identification Profile (SIP) is developed to represent the Identification parameters of the substance described in line with the Substance Identification requirements of REACH Annex VI and relevant guidance for the purpose of identifying the registered substance and the provision of a '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)	10031-30-8, 65996-95-4	
	synonyms	Monocalcium Phosphate (MCP), Monobasic Calcium Phosphate, Triple Super Phosphate	
	SMILES	OP(=O)(O)[O-].OP(=O)(O)[O-].[Ca+2]	
	Molecular formula	Ca2(H2PO4)2 or Ca.2H3O4P or CaH4O8P2	
	Structural image / diagram (indicative)		
	EU food legislation number / INS n°	E341i	
	State / form	Solid: Particulate / Powder	
	Granulometry range	Ca. 100% of particles have a diameter of <100µm	The substance is considered to be inhalable. Nano forms (in accordance with COMMISSION REGULATION (EU) 2018/1881 of 3 December 2018 on the definition of nanomaterial) have not been identified.
	pH range for aqueous solutions	The pH of the solution observed in the water solubility study was pH 2.4	
2.1.B	**Substances (with core identifiers) also falling under this substance (with justification)**		



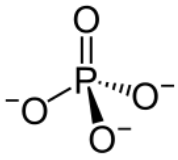
Inorganic Phosphates REACH Consortium

	Name or other Identifiers of the substance	Not applicable	
2.3	**Chemical Composition of the substance**		
2.3.1	**Main Constituent**		
	Name	Calcium bis(dihydrogenorthophosphate)	
	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)	<15%	
	Concentration range (%w/w) -Impurity (1)	≥0 < 15%	
	Relevant for classification and labelling?	N	
2.3.2.2	Name -Impurity (2)	Calcium sulphate	
	CAS Number -Impurity (2)	7778-18-9	
	EC Number -Impurity (2)	231-900-3	
	Molecular Formula -Impurity (2)	Ca.H2O4S	
	Typical concentration (%w/w) -Impurity (2)	<10%	
	Concentration range (%w/w) -Impurity (2)	≥0 < 10%	
	Relevant for classification and labelling?	N	
2.3.2.3	Name -Impurity (3)	Mineral phosphate rock	
	CAS Number -Impurity (3)	1306-05-4	
	EC Number -Impurity (3)	215-144-1	
	Molecular Formula -Impurity (3)	N/A	
	Typical concentration (%w/w) -Impurity (3)	<10%	
	Concentration range (%w/w) -Impurity (3)	≥0 < 10%	
	Relevant for classification and labelling?	N	



Inorganic Phosphates REACH Consortium

2.3.2.4	Name -Impurity (4)	Orthophosphoric acid	
	CAS Number -Impurity (4)	7664-38-2	
	EC Number -Impurity (4)	231-633-2	
	Molecular Formula -Impurity (4)	H3O4P	
	Typical concentration (%w/w) -Impurity (4)	<5%	
	Concentration range (%w/w) -Impurity (4)	≥0 < 10%	
	Relevant for classification and labelling?	N	
2.3.2.5	Name -Impurity (5)	Iron orthophosphate	
	CAS Number -Impurity (5)	10045-86-0	
	EC Number -Impurity (5)	233-149-7	
	Molecular Formula -Impurity (5)	Fe.H3O4P	
	Typical concentration (%w/w) -Impurity (5)	<5%	
	Concentration range (%w/w) -Impurity (5)	≥0 < 10%	
	Relevant for classification and labelling?	N	
2.3.2.6	Name -Impurity (6)	Magnesium Salts - various mixture	Mixture of the following: - magnesium hydrogenorthophosphate (EC 231-823-5) - Magnesium hexafluorosilicate (EC 241-022-2) -Magnesium bis (dihydrogenorthophosphate) (EC 236-004-6)
	CAS Number -Impurity (6)		
	EC Number -Impurity (6)		
	Molecular Formula -Impurity (6)		
	Typical concentration (%w/w) -Impurity (6)	<6%	
	Concentration range (%w/w) -Impurity (6)	≥0 < 10%	
	Relevant for classification and labelling?	N	
2.3.2.7	Name -Impurity (7)	Aluminium orthophosphate	
	CAS Number -Impurity (7)	7784-30-7	
	EC Number -Impurity (7)	232-056-9	
	Molecular Formula -Impurity (7)	Al.3HO3P	
	Typical concentration (%w/w) -Impurity (7)	<2%	
	Concentration range (%w/w) -Impurity (7)	≥0 < 2%	
	Relevant for classification and labelling?	N	
2.3.2.8	Name -Impurity (8)	Calcium carbonate	



Inorganic Phosphates REACH Consortium

	CAS Number -Impurity (8)	471-34-1	
	EC Number -Impurity (8)	207-439-9	
	Molecular Formula -Impurity (8)	CaCO3	
	Typical concentration (%w/w) -Impurity (8)	<4%	
	Concentration range (%w/w) -Impurity (8)	≥0 < 5%	
	Relevant for classification and labelling?	N	
2.3.2.9	Name -Impurity (9)	Other impurities	Includes Mineral insoluble residues, and other minor impurities
	CAS Number -Impurity (9)	n/a	
	EC Number -Impurity (9)	n/a	
	Molecular Formula -Impurity (9)	n/a	
	Typical concentration (%w/w) -Impurity (9)	<2.5%	
	Concentration range (%w/w) -Impurity (9)	≥0 < 2.5%	
	Relevant for classification and labelling?	N	

2.4	**Classification and labelling**
Yes - see ECHA Chem website	
2.5	**Justification for deviation from substance identity rules**

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:
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
2. The range of concentrations for the main constituent and the impurities overlap the 80% criterion and the main constituent is only occasionally ≤ 80%.