

Monoisobutyl phthalic acid

Chemical Properties

CAS No. :	30833-53-5
Formula:	C ₁₂ H ₁₄ O ₄
Molecular Weight:	222.24
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year <small>Actual storage temperature shall be subject to the COA.</small>

Biological Description

Description	Monoisobutyl phthalic acid is a phthalic acid monoester obtained by formal condensation of one of the carboxy groups of phthalic acid with the hydroxy group of isobutanol. Monoisobutyl phthalic acid functions as a human xenobiotic metabolite and a human urinary metabolite and is functionally related to isobutanol. Monoisobutyl phthalic acid is relevant in toxicological, environmental exposure, and metabolomic investigations focused on phthalate-associated biological responses and xenobiotic metabolism.
Targets(IC50)	Endogenous Metabolite

Solubility Information

Solubility	Methanol: Soluble (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	4.4996 mL	22.4982 mL	44.9964 mL
5 mM	0.8999 mL	4.4996 mL	8.9993 mL
10 mM	0.450 mL	2.2498 mL	4.4996 mL
50 mM	0.090 mL	0.450 mL	0.8999 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Kato K, et al. Quantifying phthalate metabolites in human meconium and semen using automated off-line solid-phase extraction coupled with on-line SPE and isotope-dilution high-performance liquid chromatography--tandem mass spectrometry. Anal Chem. 2006 Sep 15;78(18):6651-5.

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