

Product Data Sheet

Product Name: Phthalic acid mono-2-ethylhexyl ester

Cat. No.: GC36902

Chemical Properties

Cas. No. 4376-20-9

SMILES O=C(O)C1=CC=CC=C1C(OCC(CC)CCCC)=O

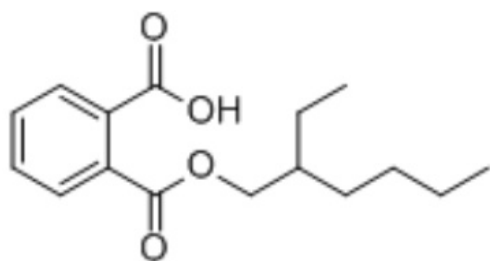
Formula $C_{16}H_{22}O_4$ M.Wt 278.34

Solubility Water: 100 mg/mL (359.27 mM); Storage Store at -20°C
DMSO: ≥ 100 mg/mL (359.27 mM)

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Cell experiment [1]:

Cell lines Human TK6 lymphoblast cells

Caution: Product has not been fully validated for medical applications. For research use only.

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The human TK6 lymphoblast cells were cultured in RPMI 1640 medium containing 10% fetal bovine serum until confluence. The cell culture was conducted under conditions of 37°C and 5% CO₂. TK6 cells were cultured at a Preparation Method density of 1×10^6 cells per 3.5ml of medium in 25cm² culture flasks. Cells were exposed to different concentrations of Phthalic acid mono-2-ethylhexyl ester (10, 50, 100, 200, 300, 400, and 500µM) for 24, 48, and 72 hours, respectively. Cell viability was determined by trypan blue exclusion.

Reaction Conditions 10, 50, 100, 200, 300, 400, and 500µM; 24, 48, and 72h

Applications Phthalic acid mono-2-ethylhexyl ester treatment inhibited cell viability of TK6 lymphoblast cells in a dose- and time-dependent manner.

Animal experiment [2]:

Animal models C57Bl/6 mice

C57Bl/6 mice were housed under controlled photoperiod conditions (lights on 08:00–20:00) with ad libitum access to tap water and a soy and alfalfa-free breeding diet. Male mice were caged with females overnight and the day following overnight mating was counted as 0.5 days post coitum (dpc).

Preparation Method 720mg/kg Phthalic acid mono-2-ethylhexyl ester was administered by oral gavage (360mg/kg twice a day at 08:30 and 18:30) to pregnant females at 13.5dpc for 24h. Pregnant mice were then killed by cervical dislocation at 14.5dpc, fetuses quickly removed and dissected under a binocular microscope. Extract the testicles from the male mouse fetal testis for analysis.

Dosage form 360mg/kg twice a day for 24h; p.o.

Applications Phthalic acid mono-2-ethylhexyl ester treatment loss of germ cells in the mouse fetal testis.

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- [1] Rosado-Berrios C A, Vélez C, Zayas B. Mitochondrial permeability and toxicity of diethylhexyl and monoethylhexyl phthalates on TK6 human lymphoblasts cells[J]. Toxicology in Vitro, 2011, 25(8): 2010-2016.
- [2] Muczynski V, Cravedi J P, Lehraiki A, et al. Effect of mono-(2-ethylhexyl) phthalate on human and mouse fetal testis: In vitro and in vivo approaches[J]. Toxicology and applied pharmacology, 2012, 261(1): 97-104.

Background

Phthalic acid mono-2-ethylhexyl ester, a major bioactive metabolite of diethylhexyl phthalate (DEHP), exhibiting anti-estrogenic ($IC_{50}=125\mu M$) and anti-androgenic effects ($IC_{50}=736\mu M$) [1]. Phthalic acid mono-2-ethylhexyl ester impairs DNA methylation, histone modifications and levels of miRNAs and lncRNAs induce alterations in several placental functions[2]. Phthalic acid mono-2-ethylhexyl ester has been widely used to decrease estradiol and progesterone production in preovulatory granulosa cells[3].

In vitro, Phthalic acid mono-2-ethylhexyl ester treatment for 72h significantly inhibited the viability of TK6 cells, with an IC_{50} value of $80\mu M$ [4]. Treatment with $100\mu M$ Phthalic acid mono-2-ethylhexyl ester for 24 hours significantly increased the triglyceride levels in HepG2 cells, upregulated the expression of SREBP-1c and ChREBP genes, and enhanced the protein expressions of ChREBP1, ACC, FAS and SCD[5]. Treatment with $200\mu M$ Phthalic acid mono-2-ethylhexyl ester for 24 hours significantly inhibited the invasion of HTR-8/SVneo cells and activated the PPAR γ pathway[6]. Phthalic acid mono-2-ethylhexyl ester ($100\mu M$; 36h) induced apoptosis in p53-silenced L02 cells, along with the up-regulations of Fas and FasL proteins as well as increased the Bax/Bcl-2 ratio and Caspase 3, 8, and 9 activities[7].

In vivo, Phthalic acid mono-2-ethylhexyl ester was administered to pregnant female mice for 24 hours by intragastric administration ($360mg/kg$; twice daily; at 08:30 and 18:30, respectively), which resulted in the loss of germ cells in the testes of the fetal mice, and the apoptosis rate significantly increased[8].

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- [1] Kim D H, Park C G, Kim S H, et al. The effects of mono-(2-ethylhexyl) phthalate (MEHP) on human estrogen receptor (hER) and androgen receptor (hAR) by YES/YAS in vitro assay[J]. *Molecules*, 2019, 24(8): 1558.
- [2] Martínez-Razo L D, Martínez-Ibarra A, Vázquez-Martínez E R, et al. The impact of Di-(2-ethylhexyl) Phthalate and Mono (2-ethylhexyl) Phthalate in placental development, function, and pathophysiology[J]. *Environment International*, 2021, 146: 106228.
- [3] Reinsberg J, Wegener-Topper P, van der Ven K, et al. Effect of mono-(2-ethylhexyl) phthalate on steroid production of human granulosa cells[J]. *Toxicology and applied pharmacology*, 2009, 239(1): 116-123.
- [4] Rosado-Berrios C A, Vélez C, Zayas B. Mitochondrial permeability and toxicity of diethylhexyl and monoethylhexyl phthalates on TK6 human lymphoblasts cells[J]. *Toxicology in Vitro*, 2011, 25(8): 2010-2016.
- [5] Bai J, He Z, Li Y, et al. Mono-2-ethylhexyl phthalate induces the expression of genes involved in fatty acid synthesis in HepG2 cells[J]. *Environmental Toxicology and Pharmacology*, 2019, 69: 104-111.
- [6] Gao F, Hu W, Li Y, et al. Mono-2-ethylhexyl phthalate inhibits human extravillous trophoblast invasion via the PPAR γ pathway[J]. *Toxicology and applied pharmacology*, 2017, 327: 23-29.
- [7] Yang G, Zhang W, Qin Q, et al. Mono (2-ethylhexyl) phthalate induces apoptosis in p53-silenced L02 cells via activation of both mitochondrial and death receptor pathways[J]. *Environmental Toxicology*, 2015, 30(10): 1178-1191.
- [8] Muczynski V, Cravedi J P, Lehraiki A, et al. Effect of mono-(2-ethylhexyl) phthalate on human and mouse fetal testis: In vitro and in vivo approaches[J]. *Toxicology and applied pharmacology*, 2012, 261(1): 97-104.

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