



Fasiglifam(TAK-875) Hemihydrate

Cat. No.:	OB0225WX-2505
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	5 mg; 10 mg; 50 mg; 200 mg

This product is for research use only and is not intended for diagnostic use.

Product Overview

Description	Fasiglifam (TAK-875) Hemihydrate is a high-affinity GPR40 agonist featuring an EC ₅₀ of 14 nM, making it approximately 400 times more potent than oleic acid in human GPR40-expressing cells.
Synonym	1374598-80-7; Fasiglifam hemihydrate; TAK875; (3S)-6-((2',6'-Dimethyl-4'-(3-(methylsulfonyl)propoxy) biphenyl-3-yl)methoxy)-2,3-dihydro-1-benzofuran-3-yl)acetic acid hemihydrate; (3S)-6-((2',6'-Dimethyl-4'-(3-(methylsulfonyl)propoxy) biphenyl-3-yl)methoxy)-2,3-dihydro-1-benzofuran-3-yl)acetic acid hydrate; 2-[(3S)-6-[[3-[2,6-dimethyl-4-(3-methylsulfonylpropoxy)phenyl]phenyl]methoxy]-2,3-dihydro-1-benzofuran-3-yl]acetic acid;hydrate; 3-Benzofuranacetic acid, 6-((2',6'-dimethyl-4'-(3-(methylsulfonyl)propoxy)(1,1'-biphenyl)-3-yl)methoxy)-2,3-dihydro-, hydrate (2:1), (3S)-; ((3S)-6-((2',6'-Dimethyl-4'-(3-(methylsulfonyl)propoxy)biphenyl-3-yl)methoxy)-2,3-dihydro-1-benzofuran-3-yl)acetic acid hemihydrate; [(3S)-6-({2',6'-Dimethyl-4'-[3-(methylsulfonyl)propoxy]biphenyl-3-yl}methoxy)-2,3-dihydro-1-benzofuran-3-yl]acetic acid hemi hydrate; 3-Benzofuranacetic acid, 6-[[2',6'-dimethyl-4'-[3-(methylsulfonyl)propoxy][1,1'-biphenyl]-3-yl]methoxy]-2,3-dihydro-, hydrate (2:1), (3S)-
CAS No.	1374598-80-7
Compound CID	57339446
Formula	C ₂₉ H ₃₂ O ₇ S·1/2H ₂ O
Formula Weight	533.63

Specification



IUPAC Name	2-[(3S)-6-[[3-[2,6-Dimethyl-4-(3-methylsulfonylpropoxy)phenyl]phenyl]methoxy]-2,3-dihydro-1-benzofuran-3-yl]acetic acid;hydrate
InChI	InChI=1S/2C29H32O7S.H2O/c2*1-19-12-25(34-10-5-11-37(3,32)33)13-20(2)29(19)22-7-4-6-21(14-22)17-35-24-8-9-26-23(15-28(30)31)18-36-27(26)16-24;/h2*4,6-9,12-14,16,23H,5,10-11,15,17-18H2,1-3H3,(H,30,31);1H2/t2*23-;/m11./s1
InChI Key	OJXYMYDDAVXPIK-IWKNALKQSA-N
SMILES string	CC1=CC(=CC(=C1C2=CC=CC(=C2)COC3=CC4=C(C=C3)[C@@H](CO4)CC(=O)O)C)OCCCS(=O)(=O)C.C1=CC(=CC(=C1C2=CC=CC(=C2)COC3=CC4=C(C=C3)[C@@H](CO4)CC(=O)O)C)OCCCS(=O)(=O)C.O
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	Fasiglifam (TAK-875) Hemihydrate is utilized in diabetes research as a selective GPR40 agonist to investigate the glucose-dependent stimulation of insulin secretion from pancreatic beta cells.

Library Information

Target	GPR
Pathways	Endocrinology & Hormones
Plate Number	L6700-04
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	100 mg/mL; 187.4 mM
ALogP	9.968
HBA_Count	12
HBD_Count	0
Rotatable Bond	22