Typical Product Specifications & Properties

PF 04418948

CAS Number: : 1078166-57-0

Specifications	Limits
Chemical Structure	chemicalStructure-pf-04418948
Molecular Formula	C23H20FNO5
Molecular weight	
Canonicalized Compound	1
Compound Complexity	629
Hydrogen Bond Acceptor Count	6
Hydrogen Bond Donor Count	1
Rotatable Bond Count	6
Allowed IUPAC Name	1-(4-fluorobenzoyl)-3-[(6-methoxy-2-naphthyl)oxymethyl]azetidine-3-carboxylic acid
CAS-like Style IUPAC Name	1-[(4-fluorophenyl)-oxomethyl]-3-[(6-methoxy-2-naphthalenyl)oxymethyl]-3-azetidinecarboxylic acid
Markup IUPAC Name	1-(4-fluorobenzoyl)-3-[(6-methoxynaphthalen-2-yl)oxymethyl]azetidine-3-carboxylic acid
Preferred IUPAC Name	1-(4-fluorobenzoyl)-3-[(6-methoxynaphthalen-2-yl)oxymethyl]azetidine-3-carboxylic acid

Specifications	Limits
Systematic IUPAC Name	1-(4-fluorophenyl)carbonyl-3-[(6-methoxynaphthalen-2-yl)oxym carboxylic acid
Traditional IUPAC Name	1-(4-fluorobenzoyl)-3-[(6-methoxy-2-naphthoxy)methyl]azetidir
Standard InChI	InChI=1S/C23H20FNO5/c1-29-19-8-4-17-11-20(9-5-16(17)10-19)3 23(22(27)28)12-25(13-23)21(26)15-2-6-18(24)7-3-15/h2-11H,12-
Standard InChIKey	LWJGMYMNSNVCEM-UHFFFAOYSA-N
XLogP3-AA Log P	3.5
Exact Mass	409.13255090
Molecular Weight	409.4
Canonical SMILES	COC1=CC2=C(C=C1)C=C(C=C2)OCC3(CN(C3)C(=O)C4=CC
Isomeric SMILES	COC1=CC2=C(C=C1)C=C(C=C2)OCC3(CN(C3)C(=O)C4=CC
Polar Surface Area Topological	76.1

Specifications	Limits
Monoisotopic Weight	409.13255090