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Typical Product Specifications & Properties

5,7-dimethyl-6-(4-methylbenzyl)pyrazolo[1,5-a]pyrimidine-3-carboxylic acid

CAS Number: : 440627-38-3

Specifications	Limits
Chemical Structure	 chemicalStructure-5-7-dimethyl-6-4-methylbenzyl-pyrazolo-1-5-a-pyrimidine-3-carboxylic-acid
Molecular Formula	C ₁₇ H ₁₇ N ₃ O ₂
Molecular weight	
Canonicalized Compound	1
Compound Complexity	409
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	1
Rotatable Bond Count	3
Allowed IUPAC Name	5,7-dimethyl-6-(p-tolylmethyl)pyrazolo[1,5-a]pyrimidine-3-carboxylic acid
CAS-like Style IUPAC Name	5,7-dimethyl-6-[(4-methylphenyl)methyl]-3-pyrazolo[1,5-a]pyrimidinecarboxylic acid
Markup IUPAC Name	5,7-dimethyl-6-[(4-methylphenyl)methyl]pyrazolo[1,5-a]pyrimidine-3-carboxylic acid
Preferred IUPAC Name	5,7-dimethyl-6-[(4-methylphenyl)methyl]pyrazolo[1,5-a]pyrimidine-3-carboxylic acid



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Specifications	Limits
Systematic IUPAC Name	5,7-dimethyl-6-[(4-methylphenyl)methyl]pyrazolo[1,5-a]pyrimidine-3-carboxylic acid
Traditional IUPAC Name	5,7-dimethyl-6-(4-methylbenzyl)pyrazolo[1,5-a]pyrimidine-3-carboxylic acid
Standard InChI	InChI=1S/C17H17N3O2/c1-10-4-6-13(7-5-10)8-14-11(2)19-16-15(17(21)22)9-18-20(16)12(14)3/h4-7,9H,8H2,1-3H3,(H,21,22)
Standard InChIKey	OMSILRKQITZRJJ-UHFFFAOYSA-N
XLogP3-AA Log P	2.9
Exact Mass	295.132076794
Molecular Weight	295.34
Canonical SMILES	<chem>CC1=CC=C(C=C1)CC2=C(N3C(=C(C=N3)C(=O)O)N=C2C)C</chem>



Specifications Limits

Isomeric SMILES

CC1=CC=C(C=C1)CC2=C(N3C(=C(C=N3)C(=O)O)N=C2C)C

Polar Surface Area

67.5

Topological

Molecular

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Monoisotopic Weight 295.132076794



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