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Typical Product Specifications & Properties

methyl 3-(hydroxymethyl)-1-methyl-1H-pyrazole-5-carboxylate

CAS Number: : 1208081-25-7

Specifications	Limits
Molecular Formula	C7H10N2O3
Molecular weight	
Canonicalized Compound	1
Compound Complexity	174
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	1
Rotatable Bond Count	3
Allowed IUPAC Name	methyl 5-(hydroxymethyl)-2-methyl-pyrazole-3-carboxylate
CAS-like Style IUPAC Name	5-(hydroxymethyl)-2-methyl-3-pyrazolecarboxylic acid methyl ester
Markup IUPAC Name	methyl 5-(hydroxymethyl)-2-methylpyrazole-3-carboxylate
Preferred IUPAC Name	methyl 5-(hydroxymethyl)-2-methylpyrazole-3-carboxylate
Systematic IUPAC Name	methyl 5-(hydroxymethyl)-2-methyl-pyrazole-3-carboxylate



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Disclaimer: this is a web generated product specification and property document. All information on this document is subject to reconfirmation at time of quote and order.




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Specifications	Limits
Traditional IUPAC Name	2-methyl-5-methylol-pyrazole-3-carboxylic acid methyl ester
Standard InChI	InChI=1S/C7H10N2O3/c1-9-6(7(11)12-2)3-5(4-10)8-9/h3,10H,4H2,1-2H3
Standard InChIKey	MZHNDLRCKWKTSU-UHFFFAOYSA-N
XLogP3-AA Log P	-0.4
Exact Mass	170.06914219
Molecular Weight	170.17
Canonical SMILES	CN1C(=CC(=N1)CO)C(=O)OC
Isomeric SMILES	CN1C(=CC(=N1)CO)C(=O)OC
Polar Surface Area Topological	64.4
Monoisotopic Weight	170.06914219
Chemical Structure	 615591 615591_methyl-3-hydroxymethyl-1-methyl-1h-pyrazole-5-carboxylate.png chemical structure

Specifications

Limits

Chemical Structure

 chemicalStructure-methyl-3-hydroxymethyl-1-methyl-1h-pyrazole-5-carboxylate

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