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Typical Product Specifications & Properties

1-(1-ETHYL-1H-PYRAZOL-4-YL)METHANAMINE

CAS Number: : 856696-09-8

Specifications	Limits
Molecular Formula	C ₆ H ₁₁ N ₃
Molecular weight	
Canonicalized Compound	1
Compound Complexity	84.4
Hydrogen Bond Acceptor Count	2
Hydrogen Bond Donor Count	1
Rotatable Bond Count	2
Allowed IUPAC Name	(1-ethylpyrazol-4-yl)methanamine
CAS-like Style IUPAC Name	(1-ethyl-4-pyrazolyl)methanamine
Markup IUPAC Name	(1-ethylpyrazol-4-yl)methanamine
Preferred IUPAC Name	(1-ethylpyrazol-4-yl)methanamine
Systematic IUPAC Name	(1-ethylpyrazol-4-yl)methanamine



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Specifications	Limits
Traditional IUPAC Name	(1-ethylpyrazol-4-yl)methylamine
Standard InChI	InChI=1S/C6H11N3/c1-2-9-5-6(3-7)4-8-9/h4-5H,2-3,7H2,1H3
Standard InChIKey	MIAQYVFWXDEYAK-UHFFFAOYSA-N
XLogP3-AA Log P	-0.6
Exact Mass	125.095297364
Molecular Weight	125.17
Canonical SMILES	<chem>CCN1C=C(C=N1)CN</chem>
Isomeric SMILES	<chem>CCN1C=C(C=N1)CN</chem>
Polar Surface Area Topological	43.8
Monoisotopic Weight	125.095297364
Chemical Structure	 chemicalStructure-1-1-ethyl-1h-pyrazol-4-yl-methanamine



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