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Typical Product Specifications & Properties

(but-3-yn-1-yl)dimethylamine

CAS Number: : 14731-37-4

Specifications	Limits
Molecular Formula	C ₆ H ₁₁ N
Molecular weight	
Canonicalized Compound	1
Compound Complexity	75.4
Hydrogen Bond Acceptor Count	1
Hydrogen Bond Donor Count	
Rotatable Bond Count	2
Allowed IUPAC Name	N,N-dimethylbut-3-yn-1-amine
CAS-like Style IUPAC Name	N,N-dimethyl-3-butyn-1-amine
Markup IUPAC Name	N,N-dimethylbut-3-yn-1-amine
Preferred IUPAC Name	N,N-dimethylbut-3-yn-1-amine
Systematic IUPAC Name	N,N-dimethylbut-3-yn-1-amine



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Specifications	Limits
Traditional IUPAC Name	but-3-ynyl(dimethyl)amine
Standard InChI	InChI=1S/C6H11N/c1-4-5-6-7(2)3/h1H,5-6H2,2-3H3
Standard InChIKey	WSCWSMUKWIYUFV-UHFFFAOYSA-N
XLogP3-AA Log P	0.8
Exact Mass	97.089149355
Molecular Weight	97.16
Canonical SMILES	CN(C)CCC#C
Isomeric SMILES	CN(C)CCC#C
Polar Surface Area Topological	3.2
Monoisotopic Weight	97.089149355
Chemical Structure	 chemicalStructure-but-3-yn-1-yl-dimethylamine



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