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Typical Product Specifications & Properties

Benzenesulfonamide, 4-nitro-N-propyl-

CAS Number: : 23530-47-4

Specifications	Limits
Molecular Formula	C9H12N2O4S
Molecular weight	
Canonicalized Compound	1
Compound Complexity	322
Hydrogen Bond Acceptor Count	5
Hydrogen Bond Donor Count	1
Rotatable Bond Count	4
Allowed IUPAC Name	4-nitro-N-propyl-benzenesulfonamide
CAS-like Style IUPAC Name	4-nitro-N-propylbenzenesulfonamide
Markup IUPAC Name	4-nitro- N -propylbenzenesulfonamide
Preferred IUPAC Name	4-nitro-N-propylbenzenesulfonamide
Systematic IUPAC Name	4-nitro-N-propyl-benzenesulfonamide



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Specifications	Limits
Traditional IUPAC Name	4-nitro-N-propyl-benzenesulfonamide
Standard InChI	InChI=1S/C9H12N2O4S/c1-2-7-10-16(14,15)9-5-3-8(4-6-9)11(12)13/h3-6,10H,2,7H2,1H3
Standard InChIKey	WPVVWLXGHXMNMA-UHFFFAOYSA-N
XLogP3-AA Log P	1.6
Exact Mass	244.05177804
Molecular Weight	244.27
Canonical SMILES	<chem>CCCNS(=O)(=O)C1=CC=C(C=C1)[N+](=O)[O-]</chem>
Isomeric SMILES	<chem>CCCNS(=O)(=O)C1=CC=C(C=C1)[N+](=O)[O-]</chem>
Polar Surface Area Topological	100
Monoisotopic Weight	244.05177804
Chemical Structure	 chemicalStructure-benzenesulfonamide-4-nitro-n-propyl-



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