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Typical Product Specifications & Properties

Potassium (S)-oxirane-2-carboxylate

CAS Number: : 82079-45-6

Specifications	Limits
Chemical Structure	 chemicalStructure-potassium-s-oxirane-2-carboxylate
Molecular Formula	C3H3KO3
Molecular weight	
Canonicalized Compound	1
Compound Complexity	82.2
Hydrogen Bond Acceptor Count	3
Hydrogen Bond Donor Count	
Rotatable Bond Count	1
Allowed IUPAC Name	potassium;(2S)-oxirane-2-carboxylate
CAS-like Style IUPAC Name	potassium;(2S)-2-oxiranecarboxylate
Markup IUPAC Name	potassium;(2<l>S</l>)-oxirane-2-carboxylate
Preferred IUPAC Name	potassium;(2S)-oxirane-2-carboxylate



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Specifications	Limits
Systematic IUPAC Name	potassium;(2S)-oxirane-2-carboxylate
Traditional IUPAC Name	potassium;(2S)-oxirane-2-carboxylate
Standard InChI	InChI=1S/C3H4O3.K/c4-3(5)2-1-6-2;/h2H,1H2,(H,4,5);/q:+1/p-1/t2-;/m0./s1
Standard InChIKey	CMQCDPNYSJUSEH-DKWTVANSSA-M
Exact Mass	125.97192544
Molecular Weight	126.15
Canonical SMILES	C1C(O1)C(=O)[O-].[K+]
Isomeric SMILES	C1[C@H](O1)C(=O)[O-].[K+]
Polar Surface Area Topological	52.7
Monoisotopic Weight	125.97192544



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