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Typical Product Specifications & Properties

L-Sinigrin Monohydrate

CAS Number: : 3952-98-5

Specifications	Limits
Molecular weight	397.46
EINECS	223-545-8
SMILES	[K+].OC[C@H]1O[C@@H](S\C(=N/OS(=O)(=O)[O-])\CC=C)[C@H](O)[C@@H](O)[C@@H]1O
InChI	QKFAFSGJTMHRRY-FVDOMRANSA-M
InChIKey	1S/C10H17NO9S2.K/c1-2-3-6(11-20-22(16,17)18)21-10-9(15)8(14)7(13)5(4-12)19-10;/h2,5,7-10,12-15H,1,3-4H2,(H,16,17,18);/q:+1/p-1/b11-6-;/t5-,7-,8+,9-,10+;/m1./s1
Atmospheric OH Rate Constant	1.96E-10 cm ³ /molecule-sec
log P (octanol-water)	-4.180



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