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Typical Product Specifications & Properties

Trinexapac-Ethyl

CAS Number: : 95266-40-3

Specifications	Limits
Molecular weight	252.26
EINECS	1308068-626-2
SMILES	<chem>C1CC1\C(O)=C1/C(=O)CC(C(=O)OCC)CC1=O</chem>
InChI	RVKCCVTVZORVGD-QXMHVHEDSA-N
InChIKey	1S/C13H16O5/c1-2-18-13(17)8-5-9(14)11(10(15)6-8)12(16)7-3-4-7/h7-8,16H,2-6H2,1H3/b12-11-
Vapor Pressure	1.62E-05 mm Hg
pKa Dissociation Constant	4.57
Water solubility	2.8 mg/L
Henry's Law Constant	1.92E-06 atm-m ³ /mole
Melting Point	36 °C
Atmospheric OH Rate Constant	9.51E-11 cm ³ /molecule-sec
log P (octanol-water)	1.6



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Specifications	Limits
Refractive Index	nD30 1.5350
Melting Point	32-36°C



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