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Typical Product Specifications & Properties

Benzyl nicotinate

CAS Number: : 94-44-0

Specifications	Limits
Molecular weight	213.23
SMILES	<chem>c1(C(OCc2ccccc2)=O)ccncc1</chem>
InChI	1S/C13H11NO2/c15-13(12-7-4-8-14-9-12)16-10-11-5-2-1-3-6-11/h1-9H,10H2
InChIKey	KVYGGMBOZFWZBQ-UHFFFAOYSA-N
log P (octanol-water)	2.4
Water solubility	333 mg/L
Henry's Law Constant	3.67E-09 atm-m ³ /mole
Atmospheric OH Rate Constant	6.46E-12 cm ³ /molecule-sec
Vapor Pressure	1.16E-04 mm Hg



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