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Typical Product Specifications & Properties

1-[(dimethylamino)methyl]-1-methylpropyl benzoate

CAS Number: : 644-26-8

Specifications	Limits
Molecular weight	235.32
EINECS	211-411-1
SMILES	<chem>CCC(C)(CN(C)C)OC(=O)c1ccccc1</chem>
InChI	FDMBBCOBEAVDAO-UHFFFAOYSA-N
InChIKey	1S/C14H21NO2/c1-5-14(2,11-15(3)4)17-13(16)12-9-7-6-8-10-12/h6-10H,5,11H2,1-4H3
log P (octanol-water)	2.890
Vapor Pressure	7.47E-04 mm Hg
Atmospheric OH Rate Constant	8.27E-11 cm ³ /molecule-sec
Henry's Law Constant	5.35E-08 atm-m ³ /mole
Water solubility	992 mg/L



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