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Typical Product Specifications & Properties

Diphenhydramine

CAS Number: : 58-73-1

Specifications	Limits
Molecular weight	255.35
EINECS	200-396-7
InChI	1S/C17H21NO/c1-18(2)13-14-19-17(15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3-12,17H,13-14H2,1-2H3
InChIKey	ZZVUWRFKOJYTH-UHFFFAOYSA-N
Henry's Law Constant	3.70E-09 atm-m3/mole
Vapor Pressure	3.70E-05 mm Hg
Melting Point	168 ° C
Atmospheric OH Rate Constant	1.27E-10 cm3/molecule-sec
pKa Dissociation Constant	8.98
log P (octanol-water)	3.27
Water solubility	3060 mg/L
Melting Point	167-172°C



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Molecular weight	255.35
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SMILES	<chem>C(c1ccccc1)(c1ccccc1)OCCN(C)C</chem>
InChI	1S/C17H21NO/c1-18(2)13-14-19-17(15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3-12,17H,13-14H2,1-2H3
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