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Typical Product Specifications & Properties

tert-Butyl Diethylphosphonoacetate

CAS Number: : 27784-76-5

Specifications	Limits
Molecular weight	252.24
Flash Point	>230 °F
Boiling Point	100-103 °C/1.5 mm Hg
BRN Number	2050126
Density	1.074 g/mL at 25 °C
Refractive Index	1.431
Water solubility	Not miscible or difficult to mix in water.
Molecular weight	150.18
EINECS	205-343-1
SMILES	<chem>c1(ccc(N=O)cc1)N(C)C</chem>
InChI	1S/C8H10N2O/c1-10(2)8-5-3-7(9-11)4-6-8/h3-6H,1-2H3
InChIKey	CMEWLCATCRTSGF-UHFFFAOYSA-N



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Specifications	Limits
pKa Dissociation Constant	4.544
Melting Point	92.5 ° C
Water solubility	1370 mg/L
log P (octanol-water)	2.040
Atmospheric OH Rate Constant	1.96E-10 cm ³ /molecule-sec
Henry's Law Constant	8.96E-07 atm-m ³ /mole
Vapor Pressure	0.406 mm Hg
Melting Point	85-87 °C
Stability	Stable. Incompatible with strong oxidizing agents, strong reducing agents, strong acids, acetic acid, acetic anhydride. Highly flammable (?)
Density	1,15 g/cm ³
BRN Number	607293
Merck	14,6638



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Specifications	Limits
Storage Temperature	Flammables area



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