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Typical Product Specifications & Properties

Benzaldehyde, Semicarbazone

CAS Number: : 1574-10-3

Specifications	Limits
Molecular weight	163.18
EINECS	216-397-0
SMILES	<chem>c1cc(\C=N\NC(=O)N)ccc1</chem>
InChI	1S/C8H9N3O/c9-8(12)11-10-6-7-4-2-1-3-5-7/h1-6H,(H3,9,11,12)
InChIKey	AKGUXECGGCUDCV-UHFFFAOYSA-N
pKa Dissociation Constant	-1.05E+00
Water solubility	5450 mg/L
Atmospheric OH Rate Constant	8.57E-12 cm ³ /molecule-sec
log P (octanol-water)	1.27
Vapor Pressure	9.81E-05 mm Hg
Henry's Law Constant	7.88E-11 atm-m ³ /mole
Chemical Structure	 60212 60212_benzaldehyde-semicarbazone.png chemical structure

