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Typical Product Specifications & Properties

(±)-1-Phenylethyl isothiocyanate

CAS Number: : 4478-92-6

Specifications	Limits
Molecular weight	163.24
SMILES	<chem>c1([C@@H](N=C=S)C)ccccc1</chem>
InChI	QQCJPTVZIZVKEZ-UHFFFAOYSA-N
InChIKey	1S/C9H9NS/c1-8(10-7-11)9-5-3-2-4-6-9/h2-6,8H,1H3
log P (octanol-water)	3.46
Vapor Pressure	0.011 mm Hg
Water solubility	73.4 mg/L
Atmospheric OH Rate Constant	6.73E-12 cm ³ /molecule-sec
Henry's Law Constant	3.33E-04 atm-m ³ /mole



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