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Typical Product Specifications & Properties

4-Dimethylaminophenyl isothiocyanate

CAS Number: : 2131-64-8

Specifications	Limits
Molecular weight	178.25
SMILES	<chem>c1cc(N(C)C)ccc1N=C=S</chem>
InChI	1S/C9H10N2S/c1-11(2)9-5-3-8(4-6-9)10-7-12/h3-6H,1-2H3
InChIKey	HRDJPEMAGYHSJR-UHFFFAOYSA-N
log P (octanol-water)	3.96
Water solubility	23.3 mg/L
Henry's Law Constant	1.24E-05 atm-m ³ /mole
Vapor Pressure	2.69E-03 mm Hg
Atmospheric OH Rate Constant	2.03E-10 cm ³ /molecule-sec



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