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Typical Product Specifications & Properties

4-Methylphenyl Isothiocyanate

CAS Number: : 622-59-3

Specifications	Limits
Molecular weight	149.21
SMILES	<chem>c1(ccc(C)cc1)N=C=S</chem>
InChI	1S/C8H7NS/c1-7-2-4-8(5-3-7)9-6-10/h2-5H,1H3
InChIKey	ABQKHKWXTUVKGF-UHFFFAOYSA-N
Henry's Law Constant	8.62E-04 atm-m ³ /mole
log P (octanol-water)	3.92
Boiling Point	237 ° C
Atmospheric OH Rate Constant	5.72E-12 cm ³ /molecule-sec
Vapor Pressure	0.030 mm Hg
Water solubility	2.84 mg/L
Melting Point	25-26 ° C



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