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Typical Product Specifications & Properties

3-Bromophenyl isothiocyanate

CAS Number: : 2131-59-1

Specifications	Limits
Molecular weight	214.08
SMILES	<chem>c1(cc(cc1)Br)N=C=S</chem>
InChI	1S/C7H4BrNS/c8-6-2-1-3-7(4-6)9-5-10/h1-4H
InChIKey	ZMGMGHNOACSMQN-UHFFFAOYSA-N
Atmospheric OH Rate Constant	7.73E-13 cm ³ /molecule-sec
Boiling Point	256 ° C
log P (octanol-water)	4.12
Water solubility	17.6 mg/L
Henry's Law Constant	3.11E-04 atm-m ³ /mole
Vapor Pressure	4.11E-03 mm Hg



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