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Typical Product Specifications & Properties

3-Aminothioanisole

CAS Number: : 1783-81-9

Specifications	Limits
Molecular weight	139.22
SMILES	<chem>c1(cc(ccc1)N)SC</chem>
InChI	1S/C7H9NS/c1-9-7-4-2-3-6(8)5-7/h2-5H,8H2,1H3
InChIKey	KCHLDNLIJVS RPK-UHFFFAOYSA-N
Atmospheric OH Rate Constant	2.01E-10 cm ³ /molecule-sec
Vapor Pressure	0.012 mm Hg
pKa Dissociation Constant	4
log P (octanol-water)	1.45
Henry's Law Constant	5.55E-08 atm-m ³ /mole
Water solubility	4870 mg/L
Chemical Structure	 44005 44005_3-aminothioanisole.png chemical structure

