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Typical Product Specifications & Properties

Benzo[b]thiophene 1,1-dioxide

CAS Number: : 825-44-5

Specifications	Limits
Molecular weight	166.20
SMILES	<chem>c1ccc2C=CS(=O)(=O)c2c1</chem>
InChI	1S/C8H6O2S/c9-11(10)6-5-7-3-1-2-4-8(7)11/h1-6H
InChIKey	FRJNKYGTHPUSJR-UHFFFAOYSA-N
Atmospheric OH Rate Constant	5.68E-11 cm ³ /molecule-sec
Henry's Law Constant	7.11E-07 atm-m ³ /mole
Water solubility	1.14E+04 mg/L
log P (octanol-water)	0.88
Vapor Pressure	1.03E-03 mm Hg



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