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Typical Product Specifications & Properties

4-Methoxybenzyl isothiocyanate

CAS Number: : 3694-57-3

Specifications	Limits
Molecular weight	179.24
SMILES	<chem>COc1ccc(CN=C=S)cc1</chem>
InChI	1S/C9H9NOS/c1-11-9-4-2-8(3-5-9)6-10-7-12/h2-5H,6H2,1H3
InChIKey	IMFQYAJJXFXVMM-UHFFFAOYSA-N
Sensitive	Moisture Sensitive
Flash Point	132-133°C/0.7mm
BRN Number	2089549
Boiling Point	170-175 °C (16 mmHg)
Density	1.0872
Storage Temperature	-20°C
Refractive Index	1.591-1.598