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Typical Product Specifications & Properties

Thiobenzoic acid

CAS Number: : 98-91-9

Specifications	Limits
Molecular weight	138.19
EINECS	202-712-9
SMILES	<chem>c1(ccccc1)C(=O)S</chem>
InChI	1S/C7H6OS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)
InChIKey	UIJGNTRUPZPVNG-UHFFFAOYSA-N
Boiling Point	122 °C/30 mm Hg
Melting Point	15-18 °C
Sensitive	Air Sensitive
Refractive Index	1.605
BRN Number	1071790
Water solubility	insoluble
Flash Point	>230 °F





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Specifications	Limits
Density	1.174 g/mL at 25 °C
Storage Temperature	2-8°C
log P (octanol-water)	1.940
Atmospheric OH Rate Constant	1.37E-11 cm ³ /molecule-sec
Melting Point	24 °C



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415 Huguenot Street, New Rochelle, New York 10801

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