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Typical Product Specifications & Properties

Thiobenzamide

CAS Number: : 2227-79-4

Specifications	Limits
Molecular weight	137.20
EINECS	218-765-6
SMILES	<chem>c1(ccccc1)C(N)=S</chem>
InChI	1S/C7H7NS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H2,8,9)
InChIKey	QIOZ LISABUUKJY-UHFFFAOYSA-N
Water solubility	Slightly soluble in water.
BRN Number	606021
Melting Point	113-117 °C
Flash Point	120°C
Color	yellow
Henry's Law Constant	3.92E-07 atm-m3/mole
Vapor Pressure	0.018 mm Hg



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Specifications	Limits
Atmospheric OH Rate Constant	2.53E-11 cm ³ /molecule-sec
log P (octanol-water)	1.49
Water solubility	4.68E+04 mg/L



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