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## Typical Product Specifications & Properties

# Sulphinepyrazolone

CAS Number: : 57-96-5

Specifications	Limits
Molecular weight	404.48
EINECS	200-357-4
SMILES	<chem>c1ccc(cc1)N2C(=O)C(C(=O)N2c3ccccc3)CCS(=O)c4ccccc4</chem>
InChI	1S/C23H20N2O3S/c26-22-21(16-17-29(28)20-14-8-3-9-15-20)23(27)25(19-12-6-2-7-13-19)24(22)18-10-4-1-5-11-18/h1-15,21H,16-17H2
InChIKey	MBGGBVCIIVRRBF-UHFFFAOYSA-N
Atmospheric OH Rate Constant	9.96E-11 cm <sup>3</sup> /molecule-sec
log P (octanol-water)	2.3
Vapor Pressure	1.65E-14 mm Hg
Water solubility	31.2 mg/L
pKa Dissociation Constant	3.25
Melting Point	136-137 °C
Henry's Law Constant	5.01E-16 atm-m <sup>3</sup> /mole



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