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Typical Product Specifications & Properties

Sulphinpyrazone

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 ³ /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 ³ /mole





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Specifications	Limits
Molecular weight	267.30
EINECS	204-858-9
SMILES	<chem>Cc1c(noc1NS(=O)(=O)c2ccc(cc2)N)C</chem>
InChI	1S/C11H13N3O3S/c1-7-8(2)13-17-11(7)14-18(15,16)10-5-3-9(12)4-6-10/h3-6,14H,12H2,1-2H3
InChIKey	NHUHCSRWZMLRLA-UHFFFAOYSA-N
Stability	Stable. Incompatible with strong oxidizin
Water solubility	<0.1 g/100 mL at 22.5 ºC
Merck	13,9041
Melting Point	195°C
Storage Temperature	2-8°C
Melting Point	191 ° C
Vapor Pressure	5.08E-08 mm Hg



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Specifications	Limits
log P (octanol-water)	1.01
Water solubility	300 mg/L
Atmospheric OH Rate Constant	3.24E-11 cm ³ /molecule-sec
Henry's Law Constant	1.06E-12 atm-m ³ /mole
Solubility	acetone: complete50 mg/ml



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