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Typical Product Specifications & Properties

Sulphanilylurea

CAS Number: : 547-44-4

Specifications	Limits
Molecular weight	215.23
EINECS	208-922-7
SMILES	<chem>c1(N)ccc(S(NC(N)=O)(=O)=O)cc1</chem>
InChI	1S/C7H9N3O3S/c8-5-1-3-6(4-2-5)14(12,13)10-7(9)11/h1-4H,8H2,(H3,9,10,11)
InChIKey	WVAKABMNNSMCDK-UHFFFAOYSA-N
Water solubility	1200 mg/L
Atmospheric OH Rate Constant	2.50E-11 cm ³ /molecule-sec
Melting Point	147 dec ° C
log P (octanol-water)	-1.000
Molecular weight	214.25
EINECS	200-345-9
SMILES	<chem>c1cc(ccc1N)S(=O)(=O)NC(=N)N</chem>



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Specifications	Limits
InChI	1S/C7H10N4O2S/c8-5-1-3-6(4-2-5)14(12,13)11-7(9)10/h1-4H,8H2,(H4,9,10,11)
InChIKey	BRBKOPJOKNSWSG-UHFFFAOYSA-N
Atmospheric OH Rate Constant	4.40E-11 cm ³ /molecule-sec
pKa Dissociation Constant	11.25
Vapor Pressure	1.47E-07 mm Hg
Melting Point	191.5 ° C
Water solubility	2200 mg/L
log P (octanol-water)	-1.22E+00
Henry's Law Constant	1.01E-15 atm-m ³ /mole
Solubility	1 M HCl: soluble50mg/mL
Merck	8908
Stability	Stable. Incompatible with strong oxidizing agents.



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Specifications	Limits
Water solubility	1g/1000mL at 25 °C
Melting Point	190-193°C
Storage Temperature	-20°C
Color	white to off-white
Form	Powder



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