

Typical Product Specifications & Properties

Sulphadimethoxine Sodium

CAS Number: : 1037-50-9

Specifications	Limits
Molecular weight	332.31
EINECS	213-859-3
SMILES	<chem>COc1cc(nc(n1)OC)[N-]S(=O)(=O)c2ccc(cc2)N.[Na+]</chem>
InChI	DQDZQHMCPUUPC-UHFFFAOYSA-N
InChIKey	1S/C12H13N4O4S.Na/c1-19-11-7-10(14-12(15-11)20-2)16-21(17,18)9-5-3-8(13)4-6-9;/h3-7H,13H2,1-2H3;/q-1;+1
Merck	8905
Storage Temperature	2-8°C
Melting Point	268 °C
Molecular weight	214.25
EINECS	200-345-9
SMILES	<chem>c1cc(ccc1N)S(=O)(=O)NC(=N)N</chem>
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)

Specifications	Limits
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.
Water solubility	1g/1000mL at 25 °C

Specifications	Limits
Melting Point	190-193°C
Storage Temperature	-20°C
Color	white to off-white
Form	Powder