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Typical Product Specifications & Properties

Phenylmercuric chloride

CAS Number: : 100-56-1

Specifications	Limits
Molecular weight	1,165.03
EINECS	240-521-2
SMILES	[Na+].[Na+].[Na+].[Na+].OCCN(CCO)c1nc(Nc2ccc(cc2)S(=O)(=O)[O-])nc(Nc3ccc(\C=C\c4ccc(Nc5nc(Nc6ccc(cc6)S(=O)(=O)[O-])nc(n5)N(CCO)CCO)cc4S(=O)(=O)[O-])c(c3)S(=O)(=O)[O-])n1
InChI	CPZFDTYTCMAAQX-MBCFVHIPSA-J
InChIKey	1S/C40H44N12O16S4.4Na/c53-19-15-51(16-20-54)39-47-35(41-27-7-11-31(12-8-27)69(57,58)59)45-37(49-39)43-29-5-3-25(33(23-29)71(63,64)65)1-2-26-4-6-30(24-34(26)72(66,67)68)44-38-46-36(48-40(50-38)52(17-21-55)18-22-56)42-28-9-13-32(14-10-28)70(60,61)62;;;;
Molecular weight	313.15
EINECS	202-865-1
SMILES	c1(ccccc1)[Hg]Cl
InChI	1S/C6H5.ClH.Hg/c1-2-4-6-5-3-1;;/h1-5H;1H;/q;+1/p-1
InChIKey	AWGTVRDHKJQFAX-UHFFFAOYSA-M
Henry's Law Constant	2.65E-04 atm-m3/mole
Water solubility	310 mg/L



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Specifications	Limits
Melting Point	251 ° C
Vapor Pressure	0.028 mm Hg
log P (octanol-water)	1.78
Atmospheric OH Rate Constant	1.95E-12 cm ³ /molecule-sec
Melting Point	248-250 °C (dec.)
Merck	14,7301
Storage Temperature	Poison room
Water solubility	Soluble in benzene, ether, pyridine. Very slightly soluble in water



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