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Typical Product Specifications & Properties

HSDB 834

CAS Number: : 100-21-0

Specifications	Limits
pKa Dissociation Constant	3.51
Atmospheric OH Rate Constant	2.75E-13 cm ³ /molecule-sec
Water solubility	15 mg/L
Henry's Law Constant	3.88E-13 atm-m ³ /mole
Melting Point	>300 ° C
log P (octanol-water)	2
Melting Point	300 °C
Water solubility	slightly soluble in water (0.017 g/L at 25°C)
BRN Number	1909333
Vapor Pressure	<0.01 mm Hg (20 °C)
Stability	Stable. Combustible. Incompatible with strong oxidizing agents.
Merck	14&9162





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Specifications	Limits
Density	1.51 g/cm ³
Storage Temperature	0-6°C
Flash Point	260°C
EINECS	202-830-0
Molecular weight	166.1308
SMILES	<chem>c1(C(O)=O)ccc(C(O)=O)cc1</chem>
InChIKey	1S/C8H6O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H&(H&9&10)(H&11&12)
InChI	KKEYFWRCBNTPAC-UHFFFAOYSA-N



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