

Typical Product Specifications & Properties

HSDB 2026

CAS Number: : 104-15-4

Specifications	Limits
log P (octanol-water)	-0.620
Water solubility	6.20E+05 mg/L
Vapor Pressure	2.70E-06 mm Hg
Henry's Law Constant	2.78E-09 atm-m ³ /mole
Melting Point	104.5 ° C
pKa Dissociation Constant	-1.34E+00
Atmospheric OH Rate Constant	1.36E-12 cm ³ /molecule-sec
Storage Temperature	Flammables area
Water solubility	soluble
Density	1.07
Melting Point	106~107?
Boiling Point	116 °C

Specifications	Limits
Refractive Index	1.3825-1.3845
Flash Point	41 °C
EINECS	203-180-0
Molecular weight	172.202
SMILES	<chem>S(c1ccc(C)cc1)(O)(=O)=O</chem>
InChIKey	1S/C7H8O3S/c1-6-2-4-7(5-3-6)11(8&9)10/h2-5H&1H3&(H&8&9&10)
InChI	JOXIMZ WYDAKGHI-UHFFFAOYSA-N