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Typical Product Specifications & Properties

Thenylchlor

CAS Number: : 96491-05-3

Specifications	Limits
Molecular weight	323.84
SMILES	<chem>Cc1cccc(c1N(Cc2c(ccs2)OC)C(=O)CCl)C</chem>
InChI	KDWQYMVPYJGPHS-UHFFFAOYSA-N
InChIKey	1S/C16H18ClNO2S/c1-11-5-4-6-12(2)16(11)18(15(19)9-17)10-14-13(20-3)7-8-21-14/h4-8H,9-10H2,1-3H3
Henry's Law Constant	8.14E-09 atm-m ³ /mole
log P (octanol-water)	3.53
Water solubility	11 mg/L
Atmospheric OH Rate Constant	1.52E-10 cm ³ /molecule-sec
Vapor Pressure	2.10E-07 mm Hg
Melting Point	73 ° C



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