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Typical Product Specifications & Properties

2,6-dibromo-4-cyanophenyl butyrate

CAS Number: : 3861-41-4

Specifications	Limits
Molecular weight	347.00
EINECS	223-374-9
SMILES	<chem>c1(OC(CCC)=O)c(cc(C#N)cc1Br)Br</chem>
InChI	PGMZYNZXIYOOHJ-UHFFFAOYSA-N
InChIKey	1S/C11H9Br2NO2/c1-2-3-10(15)16-11-8(12)4-7(6-14)5-9(11)13/h4-5H,2-3H2,1H3
Vapor Pressure	4.17E-06 mm Hg
log P (octanol-water)	3.94
Henry's Law Constant	1.75E-07 atm-m ³ /mole
Water solubility	1.520 mg/L
Atmospheric OH Rate Constant	1.75E-12 cm ³ /molecule-sec