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Typical Product Specifications & Properties

2,6-DIBROMO-4-CYANOPHENYL OCTANOATE

CAS Number: : 1689-99-2

Specifications	Limits
Molecular weight	403.11
EINECS	216-885-3
SMILES	<chem>c1(c(cc(cc1Br)C#N)Br)OC(=O)CCCCCCC</chem>
InChI	DQKWXTIYGWPGOO-UHFFFAOYSA-N
InChIKey	1S/C15H17Br2NO2/c1-2-3-4-5-6-7-14(19)20-15-12(16)8-11(10-18)9-13(15)17/h8-9H,2-7H2,1H3
Water solubility	0.08 mg/L
Melting Point	45.5 ° C
log P (octanol-water)	6.1
Vapor Pressure	4.80E-06 mm Hg
Atmospheric OH Rate Constant	7.40E-12 cm ³ /molecule-sec
Henry's Law Constant	3.19E-05 atm-m ³ /mole
pKa Dissociation Constant	4.1



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415 Huguenot Street, New Rochelle, New York 10801

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