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Typical Product Specifications & Properties

Angelicin

CAS Number: : 523-50-2

Specifications	Limits
Molecular weight	186.16
EINECS	201-480-6
SMILES	<chem>c1cc2c(cco2)c3c1ccc(=O)o3</chem>
InChI	1S/C11H6O3/c12-10-4-2-7-1-3-9-8(5-6-13-9)11(7)14-10/h1-6H
InChIKey	XDROKJSWHURZGO-UHFFFAOYSA-N
Water solubility	860 mg/L
Henry's Law Constant	6.77E-07 atm-m ³ /mole
Atmospheric OH Rate Constant	4.18E-11 cm ³ /molecule-sec
Vapor Pressure	2.24E-05 mm Hg
log P (octanol-water)	2.08
Melting Point	132-134°C
Storage Temperature	2-8°C



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415 Huguenot Street, New Rochelle, New York 10801

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