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Typical Product Specifications & Properties

Cafenstrole

CAS Number : 125306-83-4

Specifications	Limits
Molecular weight	350.44
SMILES	<chem>CCN(CC)C(=O)n1cnc(n1)S(=O)(=O)c2c(cc(cc2C)C)C</chem>
InChI	HFEJHAAIJZXXRE-UHFFFAOYSA-N
InChIKey	1S/C16H22N4O3S/c1-6-19(7-2)16(21)20-10-17-15(18-20)24(22,23)14-12(4)8-11(3)9-13(14)5/h8-10H,6-7H2,1-5H3
Atmospheric OH Rate Constant	3.08E-11 cm ³ /molecule-sec
Melting Point	115 ° C
Water solubility	2.5 mg/L
log P (octanol-water)	3.21
Henry's Law Constant	4.13E-12 atm-m ³ /mole
Vapor Pressure	2.24E-11 mm Hg



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