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Typical Product Specifications & Properties

BANISTERINE MONOHYDRATE

CAS Number: : 442-51-3

Specifications	Limits
Molecular weight	212.25
SMILES	<chem>Cc1c2c(ccn1)c3ccc(cc3[nH]2)OC</chem>
InChI	1S/C13H12N2O/c1-8-13-11(5-6-14-8)10-4-3-9(16-2)7-12(10)15-13/h3-7,15H,1-2H3
InChIKey	BXNJHAXVSOCGBA-UHFFFAOYSA-N
Melting Point	273 ° C
log P (octanol-water)	3.56
Atmospheric OH Rate Constant	2.01E-10 cm ³ /molecule-sec
Water solubility	2.680 mg/L
Vapor Pressure	6.26E-06 mm Hg
Henry's Law Constant	3.13E-11 atm-m ³ /mole



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415 Huguenot Street, New Rochelle, New York 10801

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