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Typical Product Specifications & Properties

Bucetin

CAS Number: : 1083-57-4

Specifications	Limits
Molecular weight	223.27
EINECS	214-109-8
SMILES	<chem>c1(ccc(OCC)cc1)NC(C[C@H](C)O)=O</chem>
InChI	LIAWQASKBFCRNR-UHFFFAOYSA-N
InChIKey	1S/C12H17NO3/c1-3-16-11-6-4-10(5-7-11)13-12(15)8-9(2)14/h4-7,9,14H,3,8H2,1-2H3,(H,13,15)
log P (octanol-water)	1.120
Atmospheric OH Rate Constant	4.51E-11 cm ³ /molecule-sec
Melting Point	160 ° C



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415 Huguenot Street, New Rochelle, New York 10801

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