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Typical Product Specifications & Properties

Calmagite

CAS Number: : 3147-14-6

Specifications	Limits
Molecular weight	358.37
EINECS	221-563-0
SMILES	<chem>O=S(=O)(O)c1c2c(c(\N=N\c3c(O)ccc(C)c3)c(O)c1)cccc2</chem>
InChI	VBRNLOQCBCPPHL-VHEBQXMUSA-N
InChIKey	1S/C17H14N2O5S/c1-10-6-7-14(20)13(8-10)18-19-17-12-5-3-2-4-11(12)16(9-15(17)21)25(22,23)24/h2-9,20-21H,1H3,(H,22,23,24)/b19-18+
log P (octanol-water)	3.120
Atmospheric OH Rate Constant	2.05E-11 cm ³ /molecule-sec



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