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Typical Product Specifications & Properties

Potassium butyl paraben

CAS Number: : 38566-94-8

Specifications	Limits
Molecular weight	695.59
SMILES	<chem>c12c(c(ccc1Nc1ccccc1)\N=N\c1c3c(cc(c1)S(=O)(=O)[O-])cc(S(=O)(=O)[O-])cc3O)cccc2S(=O)(=O)[O-].[Na+].[Na+].[Na+]</chem>
InChI	ADGGJQPKBDIZ MT-IXIIBAVSA-K
InChIKey	1S/C26H19N3O10S3.3Na/c30-23-14-18(41(34,35)36)12-15-11-17(40(31,32)33)13-22(25(15)23)29-28-20-9-10-21(27-16-5-2-1-3-6-16)26-19(20)7-4-8-24(26)42(37,38)39;;;/h1-14,27,30H,(H,31,32,33)(H,34,35,36)(H,37,38,39);;;/q;3*+1/p-3/b29-28+;;;
Atmospheric OH Rate Constant	1.60E-10 cm ³ /molecule-sec
log P (octanol-water)	-1.140



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