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Typical Product Specifications & Properties

Rose Bengal

CAS Number: : 24545-87-7

Specifications	Limits
SMILES	<chem>c1c2c(c-3cc(c(=O)c(c3oc2c(c(c1l)[O-])l)l)c4c(c(c(c(c4Cl)Cl)Cl)Cl)C(=O)[O-].[K+].[K+]</chem>
InChI	AZJPTIGZZTZIDR-UHFFFAOYSA-L
InChIKey	1S/C20H4Cl4I4O5.2K/c21-10-8(9(20(31)32)11(22)13(24)12(10)23)7-3-1-5(25)16(29)14(27)18(3)33-19-4(7)2-6(26)17(30)15(19)28;;/h1-2,29H,(H,31,32);;/q;2*+1/p-2
Molecular weight	394.42
EINECS	201-501-9
SMILES	<chem>c12c3c(O[C@H](C3)C(=C)C)ccc1C(=O)[C@@H]1[C@H](O2)COc2c1cc(c(c2)OC)OC</chem>
InChI	1S/C23H22O6/c1-11(2)16-8-14-15(28-16)6-5-12-22(24)21-13-7-18(25-3)19(26-4)9-17(13)27-10-20(21)29-23(12)14/h5-7,9,16,20-21H,1,8,10H2,2-4H3
InChIKey	JUVIOZPCNVVQFO-UHFFFAOYSA-N
Water solubility	0.2 mg/L
log P (octanol-water)	4.1
Atmospheric OH Rate Constant	3.29E-10 cm ³ /molecule-sec
Henry's Law Constant	1.12E-13 atm-m ³ /mole



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Specifications	Limits
Melting Point	176 ° C
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