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Typical Product Specifications & Properties

1-hydroxy-2-[(6-O-β-D-xylopyranosyl-β-D-glucopyranosyl)oxy]anthraquinone

CAS Number: : 152-84-1

Specifications	Limits
Molecular weight	534.47
EINECS	205-808-9
SMILES	<chem>O1C[C@@H](O)[C@H](O)[C@H](O)[C@@H]1OC[C@@H]1[C@@H](O)[C@@H]([C@H]([C@@H](Oc2c(c3C(c4ccccc4C(c3cc2)=O)=O)O)O1)O)O</chem>
InChI	GCGGSVAWTYHZBI-CVQRVFPNSA-N
InChIKey	1S/C25H26O13/c26-12-7-35-24(22(33)18(12)29)36-8-14-20(31)21(32)23(34)25(38-14)37-13-6-5-11-15(19(13)30)17(28)10-4-2-1-3-9(10)16(11)27/h1-6,12,14,18,20-26,29-34H,7-8H2/t12-,14-,18+,20-,21+,22-,23-,24+,25-/m1/s1
Melting Point	260 ° C
Atmospheric OH Rate Constant	1.24E-10 cm ³ /molecule-sec
log P (octanol-water)	-0.670
Chemical Structure	 155223 155223_1-hydroxy-2-6-o-β-d-xylopyranosyl-β-d-glucopyranosyl-oxy-anthraquinone.png chemical structure



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