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Typical Product Specifications & Properties

1-[4-(β-D-glucopyranosyloxy)phenyl]ethan-1-one

CAS Number: : 530-14-3

Specifications	Limits
Molecular weight	298.29
EINECS	208-473-7
SMILES	<chem>c1cc(C(=O)C)ccc1O[C@@H]1O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]1O</chem>
InChI	GOZCEKPKECLKNO-RKQHYHRCSA-N
InChIKey	1S/C14H18O7/c1-7(16)8-2-4-9(5-3-8)20-14-13(19)12(18)11(17)10(6-15)21-14/h2-5,10-15,17-19H,6H2,1H3/t10-,11-,12+,13-,14-/m1/s1
Melting Point	195.5 ° C
log P (octanol-water)	-0.820
Atmospheric OH Rate Constant	8.17E-11 cm ³ /molecule-sec
Water solubility	2.00E+04 mg/L
Alpha	D23 -88° (c = 1)
Melting Point	195°C
Storage Temperature	Hygroscopic, -20°C Freezer, Under Inert Atmosphere

