4-Nitrophenyl-«beta»-D-galacturonide, tris(trimethylsilyl) ether, trimethylsilyl ester

Inchi: InChI=1S/C24H45NO9Si4/c1-35(2,3)31-19-20(32-36(4,5)6)22(33-37(7,8)9)24(30-21(19)2

InchiKey: ZKFBDCINXMTWTO-UHFFFAOYSA-N

Formula: C24H45NO9Si4

SMILES: C[Si](C)(C)OC(=O)C1OC(Oc2ccc([N+](=O)[O-])cc2)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O

Mol. weight [g/mol]: 603.96

Physical Properties

Property code	Value	Unit	Source
log10ws	2.28		Crippen Method
logp	5.737		Crippen Method
rinpol	2837.30		NIST Webbook
rinpol	2837.30		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380158&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices