«alpha»-Idofuranose, TMS

Inchi: InChI=1S/C23H52O6Si3/c1-22(2,3)26-17(16-24-30(7,8)9)18-19(27-23(4,5)6)20(28-31(10
InchiKey: SJLZQLBWPGHMAS-XNTOXWQXSA-N
Formula: C23H52O6Si3
SMILES: CC(C)(C)OC(CO[Si](C)(C)C)C1OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C1OC(C)(C)C
Mol. weight [g/mol]: 508.91

Physical Properties

Property code	Value	Unit	Source
log10ws	0.70		Crippen Method
logp	6.002		Crippen Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
ripol	1815.00		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=R52523&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
ripol: Polar retention indices