«beta»-Idofuranose, TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-18-19(25-30(7,8)9)20(26-31(10,11)12)21(24-18
InchiKey: PLNWQGWZBNJIQM-JSXRDJHFSA-N
Formula: C21H52O6Si5
SMILES: C[Si](C)(C)OCC1OC(CO[Si](C)(C)C)(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 541.06

Physical Properties

Property code	Value	Unit	Source
logp	6.076		Crippen Method
rinpol	1858.00		NIST Webbook
ripol	1771.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R52626&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
ripol: Polar retention indices

Latest version available from:
https://www.chemeo.com/cid/46-040-6/beta-Idofuranose-TMS.pdf
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