

«beta»-Idopyranose, TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-17-18(24-29(4,5)6)19(25-30(7,8)9)20(26-31(10
InchiKey: PPFHNIVPOLWPCF-QGLKVJOYSA-N
Formula: C21H52O6Si5
SMILES: C[Si](C)(C)OCC1OC(O[Si](C)(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	6.075		Crippen Method
rinpol	1909.00		NIST Webbook
rinpol	1909.00		NIST Webbook
ripol	1841.00		NIST Webbook
ripol	1841.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R52630&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):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/21-545-3/beta-Idopyranose-TMS.pdf>

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