

«beta»-Allofuranose, TMS

Inchi: InChI=1S/C21H52O6Si5/c1-28(2,3)22-16-17(24-29(4,5)6)18-19(25-30(7,8)9)20(26-31(10
InchiKey: ZIWXPOHHTJQHTN-PFAUGDHASA-N
Formula: C21H52O6Si5
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C1OC(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
log10ws	5.66		Crippen Method
logp	6.075		Crippen Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
ripol	1843.00		NIST Webbook
ripol	1843.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R52587&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/54-165-9/beta-Allofuranose-TMS.pdf>

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