

«alpha»-D-Allose, pyranose, TMS

Inchi: InChI=1S/C20H50O6Si5/c1-27(2,3)22-16-17(23-28(4,5)6)19(25-30(10,11)12)21-20(26-3)
InchiKey: DMYXNOJXHNOHDN-WPVAHCMFSA-N
Formula: C20H50O6Si5
SMILES: C[Si](C)(C)OC1OC(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]: 527.03

Physical Properties

Property code	Value	Unit	Source
logp	6.032		Crippen Method
rinpol	1864.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R440761&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/66-513-9/alpha-D-Allose-pyranose-TMS.pdf>

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