

Arabinonic acid, pentakis-TMS

Inchi: InChI=1S/C20H50O6Si5/c1-27(2,3)22-16-17(23-28(4,5)6)18(24-29(7,8)9)19(25-30(10,11)20)15-14-13-12-11-10-9-8-7-6-5-4-3-2-1
InchiKey: HUHNYCQTXQUQCH-QRVBRYPASA-N
Formula: C₂₀H₅₀O₆Si₅
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 527.03

Physical Properties

Property code	Value	Unit	Source
log10ws	6.00		Crippen Method
logp	5.876		Crippen Method
rinpol	1835.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1812.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R100626&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/52-648-5/Arabinonic-acid-pentakis-TMS.pdf>

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