

D-(-)-Fructose, pentakis(trimethylsilyl) ether, methyloxime (anti)

Inchi: InChI=1S/C22H55NO6Si5/c1-24-23-19(17-25-30(2,3)4)21(28-33(11,12)13)22(29-34(14,15)16)35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/h1-22,24-23,19(17-25-30(2,3)4)21(28-33(11,12)13)22(29-34(14,15)16)35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100/t1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100/b1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100

InchiKey: ACDMQGXCXUQPRR-UHFFFAOYSA-N

Formula: C₂₂H₅₅NO₆Si₅

SMILES: CON=C(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 570.10

Physical Properties

Property code	Value	Unit	Source
log10ws	5.70		Crippen Method
logp	6.352		Crippen Method
rinpol	1858.60		NIST Webbook
rinpol	1858.60		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U380189&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/49-433-7/D-Fructose-pentakis-trimethylsilyl-ether-methyloxime-anti.pdf>

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