

D-(+)-Cellobiose, octakis(trimethylsilyl) ether, methyloxime (isomer 1)

Inchi: InChI=1S/C37H89NO11Si8/c1-39-38-26-29(44-52(8,9)10)33(46-54(14,15)16)32(31(45-50)12)13(47-49)11/1-8
InchiKey: KNAZTEWBFRPMHZ-UHFFFAOYSA-N
Formula: C₃₇H₈₉NO₁₁Si₈
SMILES: CON=CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(OC1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C
Mol. weight [g/mol]: 948.79

Physical Properties

Property code	Value	Unit	Source
log10ws	8.77		Crippen Method
logp	9.752		Crippen Method
rinpol	2677.20		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U380100&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/70-433-3/D-Cellobiose-octakis-trimethylsilyl-ether-methyloxime-isomer-1.pdf>

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