

D-glucose, TMS diethyldithioacetal derivative

Inchi: InChI=1S/C25H62O5S2Si5/c1-18-31-25(32-19-2)24(30-37(15,16)17)23(29-36(12,13)14)
InchiKey: CNMNOZHMKGENSD-JLLPCOHGSA-N
Formula: C25H62O5S2Si5
SMILES: CCSC(SCC)C(O[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)
Mol. weight [g/mol]: 647.31

Physical Properties

Property code	Value	Unit	Source
log10ws	3.20		Crippen Method
logp	8.551		Crippen Method
rinpol	2353.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R502775&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/28-952-4/D-glucose-TMS-diethyldithioacetal-derivative.pdf>

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