

lactitol, TMS

Inchi: InChI=1S/C39H96O11Si9/c1-51(2,3)40-28-31-35(47-56(16,17)18)37(49-58(22,23)24)38(59-60(61,62)63)64
InchiKey: DTONBTAGJKRSDD-HBGKNYCSSA-N
Formula: C39H96O11Si9
SMILES: C[Si](C)(C)OCC(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
Mol. weight [g/mol]: 993.94

Physical Properties

Property code	Value	Unit	Source
log10ws	10.04		Crippen Method
logp	10.972		Crippen Method
rinpol	2894.90		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R488961&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/32-940-2/lactitol-TMS.pdf>

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