

LACTULOSE (8TMS)

Other names: Lactulose, TMS
Inchi: InChI=1S/C36H86O11Si8/c1-48(2,3)37-25-28-30(43-51(10,11)12)32(44-52(13,14)15)33(16,17)18-20-21-22-23-24-26-27-29-31-34-35-36
InchiKey: GAHZLIHEAJXJMO-KBFWXCHHSA-N
Formula: C₃₆H₈₆O₁₁Si₈
SMILES: C[Si](C)(C)OCC1OC(OC2C(CO[Si](C)(C)C)OC(CO[Si](C)(C)C)(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]: 919.75

Physical Properties

Property code	Value	Unit	Source
log10ws	8.95		Crippen Method
logp	9.478		Crippen Method
rinpol	2697.00		NIST Webbook
rinpol	2691.70		NIST Webbook
rinpol	2698.10		NIST Webbook
rinpol	2691.70		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=R154495&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/13-703-6/LACTULOSE-8TMS.pdf>

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