

meso-inositol, TMS

Inchi: InChI=1S/C24H60O6Si6/c1-31(2,3)25-19-20(26-32(4,5)6)22(28-34(10,11)12)24(30-36(13,14)16)21(27-33(7,8)9)17(18,15)11
InchiKey: FRTKXRNTVMCAKI-HPEVMFQJSA-N
Formula: C₂₄H₆₀O₆Si₆
SMILES: C[Si](C)(C)OC1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 613.24

Physical Properties

Property code	Value	Unit	Source
log10ws	6.74		Crippen Method
logp	7.321		Crippen Method
rinpol	2154.30		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R489013&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/67-045-8/meso-inositol-TMS.pdf>

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