

Xanthine riboside, TMS

Inchi: InChI=1S/C25H54N4O6Si5/c1-36(2,3)30-16-18-20(32-37(4,5)6)21(33-38(7,8)9)24(31-18)
InchiKey: VETZYJFLEMJLSG-PRYKOTLMSA-N
Formula: C25H54N4O6Si5
SMILES: C[Si](C)(C)OCC1OC(N2C=NC3=C(O[Si](C)(C)C)N=C(O[Si](C)(C)C)NC32)C(O[Si](C)(C)C)
Mol. weight [g/mol]: 647.15

Physical Properties

Property code	Value	Unit	Source
log10ws	4.79		Crippen Method
logp	5.504		Crippen Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		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=R95484&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/48-859-6/Xanthine-riboside-TMS.pdf>

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