

Saccharopine, TMS # 2

Inchi: InChI=1S/C23H52N2O6Si4/c1-32(2,3)25-20(23(28)31-35(10,11)12)15-13-14-18-24-19(2)
InchiKey: AXPOYPHOYWZNIU-UHFFFAOYSA-N
Formula: C23H52N2O6Si4
SMILES: C[Si](C)(C)NC(CCCCNC(CCC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 565.01

Physical Properties

Property code	Value	Unit	Source
log10ws	3.16		Crippen Method
logp	4.823		Crippen Method
rinpol	2526.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401553&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/99-184-9/Saccharopine-TMS-2.pdf>

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