

Saccharopine, TMS # 1

Inchi: InChI=1S/C20H44N2O6Si3/c1-29(2,3)26-18(23)14-13-17(20(25)28-31(7,8)9)22-15-11-10
InchiKey: WBNZXSJGLOMBOE-UHFFFAOYSA-N
Formula: C20H44N2O6Si3
SMILES: C[Si](C)(C)OC(=O)CCC(NCCCC(N)C(=O)O[Si](C)(C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 492.83

Physical Properties

Property code	Value	Unit	Source
log10ws	2.22		Crippen Method
logp	3.357		Crippen Method
rinpol	2427.00		NIST Webbook
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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=R401548&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/95-353-5/Saccharopine-TMS-1.pdf>

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