

Djenkolic acid, TMS

Inchi: InChI=1S/C19H46N2O4S2Si4/c1-28(2,3)20-16(18(22)24-30(7,8)9)13-26-15-27-14-17(21)
InchiKey: CIPDTUSMYWZMOW-UHFFFAOYSA-N
Formula: C19H46N2O4S2Si4
SMILES: C[Si](C)(C)NC(CSCSCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 543.05

Physical Properties

Property code	Value	Unit	Source
log10ws	3.43		Crippen Method
logp	4.753		Crippen Method
rinpol	2458.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94553&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/24-186-9/Djenkolic-acid-TMS.pdf>

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