

alloxanthine, TMS

Inchi:	InChI=1S/C26H54N4O8Si6/c1-39(2,3)33-21-25(37-43(13,14)15,19(31)27-23(29-21)35-4
InchiKey:	CRSCKJCQFDNQDS-UHFFFAOYSA-N
Formula:	C26H54N4O8Si6
SMILES:	C[Si](C)(C)OC1=NC(=O)C(O[Si](C)(C)C)(C2(O[Si](C)(C)C)C(=O)N=C(O[Si](C)(C)C)N=C
Mol. weight [g/mol]:	719.24

Physical Properties

Property code	Value	Unit	Source
log10ws	7.27		Crippen Method
logp	6.162		Crippen Method
rinpol	1843.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R305034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/12-737-0/alloxanthine-TMS.pdf>

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