

Allantoin, TMS

Inchi: InChI=1S/C16H38N4O3Si4/c1-24(2,3)20-16(23-27(10,11)12)18-13-14(21-25(4,5)6)19-15
InchiKey: DYROHQDXFXZYDA-UHFFFAOYSA-N
Formula: C16H38N4O3Si4
SMILES: C[Si](C)(C)NC(=NC1N=C(O[Si](C)(C)C)N=C1O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 446.84

Physical Properties

Property code	Value	Unit	Source
log10ws	4.35		Crippen Method
logp	4.416		Crippen Method
rinpol	1902.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94094&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/73-974-0/Allantoin-TMS.pdf>

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