

Isoxanthopterin, tris(trimethylsilyl) derivative

Inchi: InChI=1S/C15H29N5O2Si3/c1-23(2,3)19-15-18-14(21)12-13(20(15)24(4,5)6)17-11(10-16)
InchiKey: PCVKIPRNPFUTPC-UHFFFAOYSA-N
Formula: C15H29N5O2Si3
SMILES: C[Si](C)(C)Nc1nc(=O)c2ncc(O[Si](C)(C)C)nc2n1[Si](C)(C)C
Mol. weight [g/mol]: 395.68

Physical Properties

Property code	Value	Unit	Source
log10ws	1.76		Crippen Method
logp	3.330		Crippen Method
rinpol	2131.60		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U334030&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/116-950-8/Isoxanthopterin-tris-trimethylsilyl-derivative.pdf>

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