

Allopurinol, TMS

Inchi: InChI=1S/C11H20N4OSi2/c1-17(2,3)15-10-9(7-14-15)11(13-8-12-10)16-18(4,5)6/h7-8H,
InchiKey: ISWPSCOFEHTTCP-UHFFFAOYSA-N
Formula: C11H20N4OSi2
SMILES: C[Si](C)(C)Oc1ncnc2c1cnn2[Si](C)(C)C
Mol. weight [g/mol]: 280.47
CAS: 51642-61-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.08		Crippen Method
logp	2.723		Crippen Method
rinpola	1611.70		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=C51642616&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/115-215-5/Allopurinol-TMS.pdf>

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