

Allonic acid, TMS

Inchi: InChI=1S/C24H60O7Si6/c1-32(2,3)26-19-20(27-33(4,5)6)21(28-34(7,8)9)22(29-35(10,11)12)31(13,14)15-16-17-18
InchiKey: IVIMVRAMMWQMHI-MLCQCVOFSA-N
Formula: C₂₄H₆₀O₇Si₆
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[S
Mol. weight [g/mol]: 629.24

Physical Properties

Property code	Value	Unit	Source
log10ws	7.08		Crippen Method
logp	7.096		Crippen Method
rinpol	1962.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R631239&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/71-673-6/Allonic-acid-TMS.pdf>

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