

Atrolactic acid, TBDMS

Inchi: InChI=1S/C21H38O3Si2/c1-19(2,3)25(8,9)23-18(22)21(7,17-15-13-12-14-16-17)24-26(10)
InchiKey: BWLSJNORQZZDTO-UHFFFAOYSA-N
Formula: C21H38O3Si2
SMILES: CC(O[Si](C)(C)C(C)(C)C)(C(=O)O[Si](C)(C)C(C)(C)C)c1cccc1
Mol. weight [g/mol]: 394.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	6.472		Crippen Method
rinpol	1970.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563963&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/17-557-5/Atrolactic-acid-TBDMS.pdf>

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