

1-Cyclohexene-1-carboxylic acid, 3,4,5-tris[(trimethylsilyl)oxy]-, trimethylsilyl ester, [3R-(3«alpha»,4«alpha»,5«beta»)]-

Other names: 3,4,5-Tris(trimethylsilyloxy)-1-cyclohexanecarboxylic acid, trimethylsilyl ester
3,4,5-Tris(trimethylsilyloxy)-1-cyclohexene-1-carboxylic acid, trimethylsilyl ester

SHIKIMIC ACID (4TMS)

Inchi: InChI=1S/C19H42O5Si4/c1-25(2,3)21-16-13-15(19(20)24-28(10,11)12)14-17(22-26(4,5))

InchiKey: LMFAUEGOCMAFIW-UHFFFAOYSA-N

Formula: C19H42O5Si4

SMILES: C[Si](C)(C)OC(=O)C1=CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1

Mol. weight [g/mol]: 462.88

CAS: 55520-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	3.81		Crippen Method
logp	5.355		Crippen Method
rinpol	1809.80		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1809.80		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1846.00		NIST Webbook

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=C55520780&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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