

Dihydroxyfumaric acid, TBDMS

Inchi: InChI=1S/C29H62O6Si4/c1-25(2,3)29(13,14)36-32-23(30)21(33-37(15,16)26(4,5)6)22(34-35)28-24-27-20-19-18-17-16-15-14-13-12-11-10-9-8-7-6-5-4-3-2-1
InchiKey: GOZQZHAFNXLOAY-QURGRASLSA-N
Formula: C29H62O6Si4
SMILES: CC(C)(C)C(C)(C)[SiH2]OC(=O)C(O[Si](C)(C)C(C)(C)C)=C(O[Si](C)(C)C(C)(C)C)C(=O)O
Mol. weight [g/mol]: 619.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.23		Crippen Method
logp	8.662		Crippen Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564179&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/57-771-3/Dihydroxyfumaric-acid-TBDMS.pdf>

Generated by Cheméo on 2024-04-20 03:19:55.058590028 +0000 UTC m=+15872443.979167363.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.