

(E)-3-Dihydromuconic acid, TMS

Other names: (E)-3-Hydromuconic acid, TMS
(E)-Hydroxymuconic acid, TMS

Inchi: InChI=1S/C15H30O5Si3/c1-21(2,3)18-13(12-15(17)20-23(7,8)9)10-11-14(16)19-22(4,5)6

InchiKey: GIAYEVJAHHZGNG-MRBUWEIXSA-N

Formula: C15H30O5Si3

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

Mol. weight [g/mol]: 374.65

Physical Properties

Property code	Value	Unit	Source
log10ws	2.73		Crippen Method
logp	4.034		Crippen Method
rinpol	1506.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1541.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R112951&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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