

Butanedioic acid, 2-[(tert-butyl dimethylsilyl)oxy]-, bis(tert-butyl dimethylsilyl) ester

Other names: D, L-Malic acid, O-tert-butyl dimethylsilyl- bis(tert-butyl dimethylsilyl) ester
Malic acid, tris-TBDMS

Malic acid, TBDMS

Malic acid, DMTBS

Malic acid, 3tbdms derivative

Inchi:

InChI=1S/C22H48O5Si3/c1-20(2,3)28(10,11)25-17(19(24)27-30(14,15)22(7,8)9)16-18(23)

InchiKey:

LGKDLSNIOMYKSN-UHFFFAOYSA-N

Formula:

C22H48O5Si3

SMILES:

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

Mol. weight [g/mol]:

476.87

CAS:

99461-86-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.11		Crippen Method
logp	6.864		Crippen Method
rinpol	2115.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2094.50		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=C99461866&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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