

Propanedioic acid, ethyl-, bis(tert-butyldimethylsilyl) ester

Other names:

Ethylmalonic acid, diTBDMS

Ethylmalonic acid, bis-TBDMS ester

Ethylmalonic acid, TBDMS

Ethylmalonic acid, DMTBS

Ethylmalonic acid, 2tbdms derivative

Inchi:

InChI=1S/C17H36O4Si2/c1-12-13(14(18)20-22(8,9)16(2,3)4)15(19)21-23(10,11)17(5,6)7

InchiKey:

KAWVBOVEDIKUOT-UHFFFAOYSA-N

Formula:

C17H36O4Si2

SMILES:

CCC(C(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]:

360.64

CAS:

98830-32-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.52		Crippen Method
logp	5.109		Crippen Method
rinpol	1725.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1722.00		NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C98830321&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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