

Propanedioic acid, methyl-, bis(trimethylsilyl) ester

Other names:	Methylmalonic acid (2TMS) Methylmalonic acid, di(trimethylsilyl) ester Methylmalonate, bisTMS Methylmalonic acid, bis(trimethylsilyl) ester Methylmalonic acid, diTMS Propanedioic acid, 2-methyl, bis-TMS Bis(trimethylsilyl) methylmalonate Methylmalonic acid (tms) Methylmalonic acid, bis-TMS Methylmalonate, TMS Methylmalonic acid, 2tms derivative
Inchi:	InChI=1S/C10H22O4Si2/c1-8(9(11)13-15(2,3)4)10(12)14-16(5,6)7/h8H,1-7H3
InchiKey:	LJDAAXOEMCESSS-UHFFFAOYSA-N
Formula:	C10H22O4Si2
SMILES:	CC(C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	262.45
CAS:	40333-07-1

Physical Properties

Property code	Value	Unit	Source
log10ws	2.41		Crippen Method
logp	2.379		Crippen Method
rinpol	1212.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1210.30		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1225.00		NIST Webbook

rinpol	1225.00	NIST Webbook
rinpol	1197.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1225.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40333071&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

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