

Propanedioic acid, bis(trimethylsilyl) ester

Other names:	Malonic acid, bis(trimethylsilyl) ester Malonic acid (bis-TMS) Bis(trimethylsilyl) malonate Malonic acid, di(trimethylsilyl) ester Malonic acid (2TMS) Malonic acid diTMS Malonic acid (tms) Propanedioic acid, 2tms derivative
Inchi:	InChI=1S/C9H20O4Si2/c1-14(2,3)12-8(10)7-9(11)13-15(4,5)6/h7H2,1-6H3
InchiKey:	ATCKJLDGNXGLAO-UHFFFAOYSA-N
Formula:	C9H20O4Si2
SMILES:	C[Si](C)(C)OC(=O)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	248.42
CAS:	18457-04-0

Physical Properties

Property code	Value	Unit	Source
log10ws	2.58		Crippen Method
logp	2.133		Crippen Method
rinpol	1197.00		NIST Webbook
rinpol	1217.80		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1211.00		NIST Webbook

rropol	1198.00	NIST Webbook
rropol	1221.00	NIST Webbook
rropol	1215.00	NIST Webbook
rropol	1174.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18457040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rropol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/14-349-9/Propanedioic-acid-bis-trimethylsilyl-ester.pdf>

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