

METHYLMALONIC ACID, TRIS(TRIMETHYLSILYL)-

Other names:	Methylmalonic acid, tris(trimethylsilyl)- Methylmalonic acid, tris-TMS
Inchi:	InChI=1S/C13H30O4Si3/c1-11(12(14)15-18(2,3)4)13(16-19(5,6)7)17-20(8,9)10/h1-10H3
InchiKey:	NZIQCKNREBFDLB-UHFFFAOYSA-N
Formula:	C13H30O4Si3
SMILES:	CC(C(=O)O[Si](C)(C)C)=C(O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	334.64

Physical Properties

Property code	Value	Unit	Source
logp	4.299		Crippen Method
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
tb	517.61	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40333082&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/120-163-7/METHYLMALONIC-ACID-TRIS-TRIMETHYLSILYL.pdf>

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