

O,O,O'-Tris-trimethylsilylmalonate

Other names:	Malonic acid, tris-TMS
Inchi:	InChI=1S/C12H28O4Si3/c1-17(2,3)14-11(13)10-12(15-18(4,5)6)16-19(7,8)9/h10H,1-9H3
InchiKey:	WGSJCFWDDDBQNBV-UHFFFAOYSA-N
Formula:	C12H28O4Si3
SMILES:	C[Si](C)(C)OC(=O)C=C(O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	320.60
CAS:	40333-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	3.12		Crippen Method
logp	3.909		Crippen Method
rinpol	1425.00		NIST Webbook
rinpol	1425.00		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=C40333060&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/91-170-2/O-O-O-Tris-trimethylsilylmalonate.pdf>

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