

D-(-)-Citramalic acid, tert-butyldimethylsilyl ether, bis(tert-butyldimethylsilyl) ester

Other names:	Citramalic acid, 3tbdms derivative
Inchi:	InChI=1S/C23H50O5Si3/c1-20(2,3)29(11,12)26-18(24)17-23(10,28-31(15,16)22(7,8)9)19
InchiKey:	POFABCSPTUXDJQ-UHFFFAOYSA-N
Formula:	C23H50O5Si3
SMILES:	CC(CC(=O)O[Si](C)(C)C(C)(C)C)(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	490.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.53		Crippen Method
logp	7.254		Crippen Method
rinpol	2104.90		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2104.90		NIST Webbook
rinpol	2127.00		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=U333173&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/113-980-8/D-Citramalic-acid-tert-butyldimethylsilyl-ether-bis-tert-butyldimethylsilyl-ester>

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