

Oxalacetic acid, oxime, tris-TMS

Other names:	Oxalacetic acid, oxime, TMS
Inchi:	InChI=1S/C13H29NO5Si3/c1-20(2,3)17-12(15)10-11(14-19-22(7,8)9)13(16)18-21(4,5)6/h
InchiKey:	CDENGQBJRWFTTR-UHFFFAOYSA-N
Formula:	C13H29NO5Si3
SMILES:	C[Si](C)(C)ON=C(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	363.63

Physical Properties

Property code	Value	Unit	Source
log10ws	3.62		Crippen Method
logp	3.340		Crippen Method
rinpola	1528.00		NIST Webbook
rinpola	1528.00		NIST Webbook
rinpola	1528.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R113147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/46-442-0/Oxalacetic-acid-oxime-tris-TMS.pdf>

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