

Pentanedioic acid, 3-oxo-, tris(trimethylsilyl) ester

Other names:	3-Ketoglutaric acid, TMS # 3
Inchi:	InChI=1S/C14H30O5Si3/c1-20(2,3)17-12(10-13(15)18-21(4,5)6)11-14(16)19-22(7,8)9/h1
InchiKey:	JJMFGWNTLJOELF-BENRWUELSA-N
Formula:	C14H30O5Si3
SMILES:	C[Si](C)(C)OC(=O)C=C(CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	362.64
CAS:	72361-20-7

Physical Properties

Property code	Value	Unit	Source
log10ws	3.00		Crippen Method
logp	3.868		Crippen Method
rinpol	1619.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1619.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72361207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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