

2-Ketohexanoic acid ho-tms

Other names:

2-Ketocaproic acid, oxime, bis-TMS
2-Oxohexanoic acid, oxime, bis-TMS
2-Ketocaproic acid, oxime, TMS
2-Hydroxyiminohexanoic acid, 2tms derivative

Inchi:

InChI=1S/C12H27NO3Si2/c1-8-9-10-11(13-16-18(5,6)7)12(14)15-17(2,3)4/h8-10H2,1-7H

InchiKey:

BTTUPQZJICJRCZ-UHFFFAOYSA-N

Formula:

C12H27NO3Si2

SMILES:

CCCCC(=NO[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

289.52

Physical Properties

Property code	Value	Unit	Source
log10ws	0.95		Crippen Method
logp	3.762		Crippen Method
rinpol	1332.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U332266&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

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/67-523-7/2-Ketohexanoic-acid-ho-tms.pdf>

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