

Docosanoic acid, 2-[(trimethylsilyl)oxy]-, methyl ester

Other names:

«alpha»-Hydroxybehenic acid, TMS ether, methyl ester

«alpha»-Hydroxybehenic acid, TMSi-Me

Methyl 2-hydroxydocosanoate, tms derivative

Inchi: InChI=1S/C26H54O3Si/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25(2

InchiKey: QSSVMTKWPPSPAQ-UHFFFAOYSA-N

Formula: C26H54O3Si

SMILES: CCCCCCCCCCCCCCCCCCCCCC(O[Si](C)(C)C)C(=O)OC

Mol. weight [g/mol]: 442.79

CAS: 56784-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	8.811		Crippen Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56784022&Units=SI>

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

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/87-045-6/Docosanoic-acid-2-trimethylsilyl-oxy-methyl-ester.pdf>

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