

HEXADECANOIC ACID-13C4-TMS

Inchi: InChI=1S/C19H40O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-22(2,3)4/h5-
InchiKey: HKNNSWCACQFVIK-LOYIAQTISA-N
Formula: C19H40O2Si
SMILES: CCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 328.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	6.846		Crippen Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R439048&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.cheméo.com/cid/70-418-0/HEXADECANOIC-ACID-13C4-TMS.pdf>

Generated by Cheméo on 2024-08-09 02:02:35.702680723 +0000 UTC m=+1858824.949786070.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.