5,8,11-Eicosatriynoic acid, trimethylsilyl ester

Other names: 5,8,11-Eicosatriynoic acid, tms derivative
Inchi: InChI=1S/C23H36O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)25
InchiKey: XBKDHFNKZGURLX-UHFFFAOYSA-N
Formula: C23H36O2Si
SMILES: CCCCCCCCC#CCC#CCC#CCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 372.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	6.076		Crippen Method
rinpol	2557.80		NIST Webbook
rinpol	2557.80		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333563&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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