

Docosanoic acid, trimethylsilyl ester

Other names:	Behenic acid, trimethylsilyl ester Docosanoic acid, TMS ester Docosanoic acid, TMS Behenic acid, tms derivative
Inchi:	InChI=1S/C25H52O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	BJBBFOVJCKMBAL-UHFFFAOYSA-N
Formula:	C25H52O2Si
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	412.76
CAS:	74367-36-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.20		Crippen Method
logp	9.186		Crippen Method
rinpol	2632.00		NIST Webbook
rinpol	2649.00		NIST Webbook
rinpol	2644.00		NIST Webbook
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367365&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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