

Hexanedioic acid, bis(trimethylsilyl) ester

Other names:

Adipic acid, bis(trimethylsilyl) ester
Bis(trimethylsilyl) adipate
Adipic acid (tms)
Adipic acid, di(trimethylsilyl) ester
Bis(trimethylsilyl) hexanedioate
Adipate, bis-TMS
Adipic acid, (2TMS)
Adipic acid, bis-TMS
Adipic acid, diTMS
Hexanedioic acid, di-TMS ester
Hexanedioic acid, bis-TMS ester
Hexanedioic acid, 1,6-bis(trimethylsilyl) ester
Adipate, TMS
Hexanedioic acid, TMS
Hexanedioic acid, 2tms derivative

Inchi:

InChI=1S/C12H26O4Si2/c1-17(2,3)15-11(13)9-7-8-10-12(14)16-18(4,5)6/h7-10H2,1-6H3

InchiKey:

DVGSOFSSBBKDKRU-UHFFFAOYSA-N

Formula:

C₁₂H₂₆O₄Si₂

SMILES:

C[Si](C)(C)OC(=O)CCCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

290.50

CAS:

18105-31-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.33		Crippen Method
logp	3.303		Crippen Method
rinpol	1502.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1499.00		NIST Webbook

rropol	1490.00	NIST Webbook
rropol	1492.20	NIST Webbook
rropol	1497.00	NIST Webbook
rropol	1499.00	NIST Webbook
rropol	1514.00	NIST Webbook
rropol	1522.00	NIST Webbook
rropol	1516.00	NIST Webbook
rropol	1502.00	NIST Webbook
rropol	1490.00	NIST Webbook
rropol	1510.00	NIST Webbook
rropol	1515.00	NIST Webbook
rropol	1502.00	NIST Webbook
rropol	1514.00	NIST Webbook
rropol	1492.20	NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C18105312&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
rropol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/122-863-8/Hexanedioic-acid-bis-trimethylsilyl-ester.pdf>

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