L-Isoleucine, N-(trimethylsilyl)-, trimethylsilyl ester

Other names: Isoleucine, N-(trimethylsilyl)-, trimethylsilyl ester, L-
Isoleucine, N-(trimethylsilyl)-, trimethylsilyl ester
Ile, di-TMS
Isoleucine, di-TMS
Isoleucine, bis-TMS
N,O-Bis(trimethylsilyl)isoleucine
Ile, TMS
Isoleucine, TMS
L-isoleucine, 2tms derivative

Inchi: InChI=1S/C12H29NO2Si2/c1-9-10(2)11(13-16(3,4)5)12(14)15-17(6,7)8/h10-11,13H,9H2,

InchiKey: JQJPJSDLFYVVEY-GHMZBOCLSA-N

Formula: C12H29NO2Si2

SMILES: CCC(C)C(N[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 275.54

CAS: 7483-92-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.13		Crippen Method
logp	3.204		Crippen Method
rinpol	1294.00		NIST Webbook
rinpol	1320.60		NIST Webbook
rinpol	1298.80		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1286.20		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1316.34		NIST Webbook
rinpol	1316.34		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1306.52		NIST Webbook
rinpol	1320.60		NIST Webbook
rinpol	1298.80		NIST Webbook
rinpol	1286.20		NIST Webbook
rinpol	1309.25		NIST Webbook
rinpol	1306.52		NIST Webbook

ripol	1369.55	NIST Webbook
ripol	1369.55	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7483923&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
ripol:	Polar retention indices