L-Cysteine, N,S-bis(trimethylsilyl)-, trimethylsilyl ester

Other names: Alanine, N-(trimethylsilyl)-3-[(trimethylsilyl)thio]-, trimethylsilyl ester, L-
N,O,S-Tris-(trimethylsilyl)cysteine
Cysteine, (N,O,S-trimethylsilyl)-
Cysteine (N,O,S-TMS)
Cysteine, tri-TMS
Cys, tri-TMS
Cys, TMS
L-cysteine, 3tms derivative

Inchi: InChI=1S/C12H31NO2SSi3/c1-17(2,3)13-11(10-16-19(7,8)9)12(14)15-18(4,5)6/h11,13H,

InchiKey: JRLJALOBTPYEJK-LLVKDONJSA-N

Formula: C12H31NO2SSi3

SMILES: C[Si](C)(C)NC(CS[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 337.70

CAS: 7364-50-3

Physical Properties

Property code	Value	Unit	Source
log10ws	2.95		Crippen Method
logp	3.726		Crippen Method
rinpol	1562.44		NIST Webbook
rinpol	1574.31		NIST Webbook
rinpol	1571.22		NIST Webbook
rinpol	1580.37		NIST Webbook
rinpol	1553.40		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1563.23		NIST Webbook
rinpol	1580.37		NIST Webbook
rinpol	1563.23		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1571.22		NIST Webbook
rinpol	1553.40		NIST Webbook
rinpol	1568.00		NIST Webbook
ripol	1703.19		NIST Webbook
ripol	1703.19		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7364503&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