

Homocarnosine, TMS # 2

Inchi: InChI=1S/C16H32N4O3Si2/c1-24(2,3)19-9-7-8-15(21)20-14(10-13-11-17-12-18-13)16(22)
InchiKey: LIINGKSXIJFSAZ-UHFFFAOYSA-N
Formula: C16H32N4O3Si2
SMILES: C[Si](C)(C)NCCCC(=O)NC(Cc1cnc[nH]1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 384.62

Physical Properties

Property code	Value	Unit	Source
log10ws	0.91		Crippen Method
logp	1.538		Crippen Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401013&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/125-187-6/Homocarnosine-TMS-2.pdf>

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