

t-Cinnamoylglycine TBDMS

Inchi: InChI=1S/C23H39NO3Si2/c1-22(2,3)28(7,8)26-20(17-16-19-14-12-11-13-15-19)24-18-21
InchiKey: FAEBENZYVWRDMR-XIGPTBEFSA-N
Formula: C23H39NO3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CN=C(C=Cc1ccccc1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 433.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	6.668		Crippen Method
rinpol	2460.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R277291&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/10-018-0/t-Cinnamoylglycine-TBDMS.pdf>

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