

4-Carboxyphenyl glycine, TBDMS

Inchi: InChI=1S/C21H37NO4Si2/c1-20(2,3)27(7,8)25-18(23)15-22-17-13-11-16(12-14-17)19(24)
InchiKey: ZTLISQAFYFCFIL-UHFFFAOYSA-N
Formula: C21H37NO4Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CNc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]: 423.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	5.809		Crippen Method
rinpol	2751.00		NIST Webbook
rinpol	2751.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563661&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/38-899-3/4-Carboxyphenyl-glycine-TBDMS.pdf>

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