Glycine, 2-cyclohexyl-N-benzyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C21H31NO4/c1-2-3-10-15-25-20(23)19(18-13-8-5-9-14-18)22-21(24)26-16-17-

InchiKey: DCLMTGLPLXDJBD-UHFFFAOYSA-N

Formula: C21H31NO4

SMILES: CCCCCOC(=O)C(N=C(O)OCc1ccccc1)C1CCCCC1

Mol. weight [g/mol]: 361.48

Physical Properties

Property code	Value	Unit	Source
hf	-648.02	kJ/mol	Joback Method
hvap	96.30	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.800		Crippen Method
mcvol	296.990	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook
tb	993.12	K	Joback Method
tc	1220.73	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383113&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature