Glycine, 2-cyclohexyl-N-octyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C23H43NO4/c1-3-5-7-9-10-15-19-28-23(26)24-21(20-16-12-11-13-17-20)22(25

InchiKey: CHEPWSOSZHUNBP-UHFFFAOYSA-N

Formula: C23H43NO4

SMILES: CCCCCCCCOC(O)=NC(C(=O)OCCCCCC)C1CCCCC1

Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
hf	-925.83	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.350		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	1012.20	K	Joback Method
tc	1240.97	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383129&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

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

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