Glycine, 2-cyclohexyl-N-propoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C18H33NO4/c1-4-12-23-18(21)19-16(15-10-6-5-7-11-15)17(20)22-13-8-9-14(2

InchiKey: UVAFTFGIHUYTNW-UHFFFAOYSA-N

Formula: C18H33NO4

SMILES: CCCOC(O)=NC(C(=O)OCCCC(C)C)C1CCCCC1

Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
hf	-827.91	kJ/mol	Joback Method
hvap	86.95	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.255		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	897.36	K	Joback Method
tc	1104.84	K	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383068&Units=SI

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

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

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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