

Glycine, 2-cyclohexyl-N-(but-3-en-1-yl)oxycarbonyl-, isohexyl ester

InChI: InChI=1S/C19H33NO4/c1-4-5-13-24-19(22)20-17(16-11-7-6-8-12-16)18(21)23-14-9-10-1
InChIKey: LAKQFSCITLGMMLDT-UHFFFAOYSA-N

Formula: C19H33NO4

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

Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
hf	-723.12	kJ/mol	Joback Method
hvap	88.51	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.421		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	2251.00		NIST Webbook
tb	916.92	K	Joback Method
tc	1127.16	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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