

Glycine, 2-cyclohexyl-N-(2-ethylhexyl)oxycarbonyl-, isohexyl ester

InChI: InChI=1S/C23H43NO4/c1-5-7-13-19(6-2)17-28-23(26)24-21(20-14-9-8-10-15-20)22(25)2
InChIKey: NBCIMGGNSAMIEH-UHFFFAOYSA-N

Formula: C23H43NO4

SMILES: CCCCC(CC)COC(O)=NC(C(=O)OCCCC(C)C)C1CCCCC1

Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
hf	-936.39	kJ/mol	Joback Method
hvap	97.70	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	6.062		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
tb	1011.32	K	Joback Method
tc	1238.71	K	Joback Method

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383149&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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