

Glycine, 2-cyclohexyl-N-isobutoxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C28H53NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-22-32-27(30)26(25-20-17-18-16-13)/n1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: RWXQSAYFZDKFOO-UHFFFAOYSA-N
Formula: C28H53NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(N=C(O)OCC(C)C)C1CCCCC1
Mol. weight [g/mol]: 467.72

Physical Properties

Property code	Value	Unit	Source
hf	-1034.31	kJ/mol	Joback Method
hvap	109.21	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	8.156		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
pc	744.88	kPa	Joback Method
rinpol	3056.00		NIST Webbook
tb	1126.16	K	Joback Method
tc	1403.99	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=U383105&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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