

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

Inchi: InChI=1S/C26H49NO4/c1-4-5-6-7-8-9-10-11-12-13-17-20-30-25(28)24(23-18-15-14-16-17)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: VUZQXWWSNNYLTH-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(N=C(O)OCC(C)C)C1CCCCC1
Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
hf	-993.03	kJ/mol	Joback Method
hvap	104.76	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.376		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	2856.00		NIST Webbook
tb	1080.40	K	Joback Method
tc	1334.07	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383103&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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