

Glycine, 2-cyclohexyl-N-ethoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C22H41NO4/c1-3-5-6-7-8-9-10-11-15-18-27-21(24)20(23-22(25)26-4-2)19-16-
InchiKey: XXSHHLFYRFANDL-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: CCCCCCCCCCOC(=O)C(N=C(O)OCC)C1CCCCC1
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
hf	-905.19	kJ/mol	Joback Method
hvap	96.25	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.960		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	989.32	K	Joback Method
tc	1211.54	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=U383087&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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