

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

InChI: InChI=1S/C25H47NO4/c1-4-7-9-10-11-15-19-29-24(27)23(22-17-13-12-14-18-22)26-25(28)21-20-16-12
InChIKey: JHIWLXSBBMVMNF-UHFFFAOYSA-N

Formula: C25H47NO4

SMILES: CCCCCCCCOC(=O)C(N=C(O)OCC(CC)CCCC)C1CCCCC1

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-972.39	kJ/mol	Joback Method
hvap	102.54	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.986		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	2789.00		NIST Webbook
tb	1057.52	K	Joback Method
tc	1301.33	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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