

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

InChI: InChI=1S/C25H47NO4/c1-5-9-14-20(7-3)18-29-24(27)23(22-16-12-11-13-17-22)26-25(28)
InChIKey: ROYKJNWZTDAQBR-UHFFFAOYSA-N

Formula: C₂₅H₄₇NO₄

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

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-977.67	kJ/mol	Joback Method
hvap	102.15	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.842		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	881.57	kPa	Joback Method
rinsol	2700.00		NIST Webbook
rinsol	2700.00		NIST Webbook
tb	1057.08	K	Joback Method
tc	1299.37	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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