

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

InChI: InChI=1S/C21H39NO4/c1-4-7-12-17(6-3)16-26-21(24)22-19(18-13-10-9-11-14-18)20(23)
InChIKey: SFBVDFVLXHBXTJ-UHFFFAOYSA-N

Formula: C21H39NO4

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

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-889.83	kJ/mol	Joback Method
hvap	93.63	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.426		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	966.00	K	Joback Method
tc	1182.83	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383148&Units=SI

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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