

Glycine, 2-cyclohexyl-N-(but-3-en-1-yl)oxycarbonyl-, octyl ester

InChI: InChI=1S/C21H37NO4/c1-3-5-7-8-9-13-17-25-20(23)19(18-14-11-10-12-15-18)22-21(24)
InChIKey: XOZJCHPHCLDFMN-UHFFFAOYSA-N
Formula: C21H37NO4
SMILES: C=CCCOC(O)=NC(C(=O)OCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 367.52

Physical Properties

Property code	Value	Unit	Source
hf	-759.12	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.346		Crippen Method
mcpvol	316.450	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook
tb	963.12	K	Joback Method
tc	1179.36	K	Joback Method

Sources

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=U383245&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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