

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

InChI: InChI=1S/C19H33NO4/c1-3-5-7-11-15-23-18(21)17(16-12-9-8-10-13-16)20-19(22)24-14
InChIKey: MVTLOZKWNNYQAF-UHFFFAOYSA-N

Formula: C19H33NO4

SMILES: C=CCCOC(O)=NC(=O)OCCCCC)C1CCCCC1

Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
hf	-717.84	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.566		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
tb	917.36	K	Joback Method
tc	1126.61	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=U383243&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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