

Glycine, 2-cyclohexyl-N-octyloxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C23H43NO4/c1-4-5-6-7-8-12-17-28-23(26)24-21(20-15-10-9-11-16-20)22(25)2
InchiKey: IBLRJXATZAXXGK-UHFFFAOYSA-N
Formula: C23H43NO4
SMILES: CCCCCCCCOC(O)=NC(C(=O)OCCCC(C)C)C1CCCCC1
Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
hf	-931.11	kJ/mol	Joback Method
hvap	98.08	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.206		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2650.00		NIST Webbook
tb	1011.76	K	Joback Method
tc	1239.76	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383128&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

Latest version available from:

<https://www.cheméo.com/cid/97-252-5/Glycine-2-cyclohexyl-N-octyloxycarbonyl-isoheptyl-ester.pdf>

Generated by Cheméo on 2025-12-05 19:09:26.269167328 +0000 UTC m=+4709963.799207992.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.