

Glycine, 2-cyclohexyl-N-isobutoxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C22H41NO4/c1-4-5-6-7-8-9-13-16-26-21(24)20(19-14-11-10-12-15-19)23-22(2
InchiKey:	GJFZORQZWPKPAX-UHFFFAOYSA-N
Formula:	C22H41NO4
SMILES:	CCCCCCCCCOC(=O)C(N=C(O)OCC(C)C)C1CCCCC1
Mol. weight [g/mol]:	383.57

Physical Properties

Property code	Value	Unit	Source
hf	-910.47	kJ/mol	Joback Method
hvap	95.86	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.816		Crippen Method
mcpvol	334.840	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	988.88	K	Joback Method
tc	1210.76	K	Joback Method

Sources

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=U383099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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