

Glycine, 2-cyclohexyl-N-propoxycarbonyl-, hexyl ester

Inchi:	InChI=1S/C18H33NO4/c1-3-5-6-10-14-22-17(20)16(15-11-8-7-9-12-15)19-18(21)23-13-4
InchiKey:	OCXHBULWJOUHGU-UHFFFAOYSA-N
Formula:	C18H33NO4
SMILES:	CCCCCOC(=O)C(N=C(O)OCCC)C1CCCCC1
Mol. weight [g/mol]:	327.46

Physical Properties

Property code	Value	Unit	Source
hf	-822.63	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.399		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	897.80	K	Joback Method
tc	1104.11	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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