

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

Inchi:	InChI=1S/C20H37NO4/c1-3-5-6-7-8-12-16-24-19(22)18(17-13-10-9-11-14-17)21-20(23)2
InchiKey:	AHTQJYAUOMSIJW-UHFFFAOYSA-N
Formula:	C20H37NO4
SMILES:	CCCCCCCCOC(=O)C(N=C(O)OCCC)C1CCCCC1
Mol. weight [g/mol]:	355.51

Physical Properties

Property code	Value	Unit	Source
hf	-863.91	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.180		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	943.56	K	Joback Method
tc	1155.91	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383071&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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