

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

Inchi:	InChI=1S/C24H45NO4/c1-3-5-6-7-8-9-10-11-12-16-20-28-23(26)22(21-17-14-13-15-18-2
InchiKey:	DOYHKDUYVDKVMZ-UHFFFAOYSA-N
Formula:	C24H45NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(N=C(O)OCCC)C1CCCCC1
Mol. weight [g/mol]:	411.62

Physical Properties

Property code	Value	Unit	Source
hf	-946.47	kJ/mol	Joback Method
hvap	100.70	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.740		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	1035.08	K	Joback Method
tc	1271.58	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383075&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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