

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

Inchi:	InChI=1S/C19H35NO4/c1-3-5-6-7-8-12-15-24-18(21)17(20-19(22)23-4-2)16-13-10-9-11-
InchiKey:	PDSVSQQLQKDRGI-UHFFFAOYSA-N
Formula:	C19H35NO4
SMILES:	CCCCCCCCOC(=O)C(N=C(O)OCC)C1CCCCC1
Mol. weight [g/mol]:	341.49

Physical Properties

Property code	Value	Unit	Source
hf	-843.27	kJ/mol	Joback Method
hvap	89.57	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.790		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
pc	1268.25	kPa	Joback Method
rinpol	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook
tb	920.68	K	Joback Method
tc	1129.56	K	Joback Method

Sources

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=U383084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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