

Glycine, 2-cyclohexyl-N-octyloxycarbonyl-, butyl ester

Inchi: InChI=1S/C21H39NO4/c1-3-5-7-8-9-13-17-26-21(24)22-19(18-14-11-10-12-15-18)20(23)
InchiKey: BRWOAYKSVNVBAQ-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: CCCCCCOC(O)=NC(C(=O)OCCCC)C1CCCCC1
Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-884.55	kJ/mol	Joback Method
hvap	94.02	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.570		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1111.11	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	966.44	K	Joback Method
tc	1183.21	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383126&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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