

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

Inchi: InChI=1S/C20H29NO4/c1-2-3-14-24-19(22)18(17-12-8-5-9-13-17)21-20(23)25-15-16-10
InchiKey: UHSBCOQTQCVBNJ-UHFFFAOYSA-N
Formula: C20H29NO4
SMILES: CCCCO(=O)C(N=C(O)OCc1ccccc1)C1CCCC1
Mol. weight [g/mol]: 347.45

Physical Properties

Property code	Value	Unit	Source
hf	-627.38	kJ/mol	Joback Method
hvap	94.07	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.409		Crippen Method
mcvol	282.900	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinsol	2548.00		NIST Webbook
rinsol	2548.00		NIST Webbook
tb	970.24	K	Joback Method
tc	1196.31	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383112&Units=SI>

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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