Glycine, N-benzoyl, propyl ester

Inchi: InChI=1S/C12H15NO3/c1-2-8-16-11(14)9-13-12(15)10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,
InchiKey: LIOAQKDCMGPKGK-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: CCCOC(=O)CN=C(O)c1ccccc1
Mol. weight [g/mol]: 221.25

Physical Properties

Property code	Value	Unit	Source
hf	-379.08	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.944		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
tb	745.67	K	Joback Method
tc	955.26	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=R106575&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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