Propanamide, 3-phenyl-N-butyl-

Inchi: InChI=1S/C13H19NO/c1-2-3-11-14-13(15)10-9-12-7-5-4-6-8-12/h4-8H,2-3,9-11H2,1H3,(
InchiKey: UZTVEZLZUTUCBJ-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CCCCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
hf	-154.92	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.376		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	692.26	K	Joback Method
tc	894.59	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=U407150&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