Propanamide, 3-phenyl-N-isobutyl-

Inchi: InChI=1S/C13H19NO/c1-11(2)10-14-13(15)9-8-12-6-4-3-5-7-12/h3-7,11H,8-10H2,1-2H3,
InchiKey: FNZAYDHBHNUHIQ-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CC(C)CN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
hf	-160.20	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.232		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	691.82	K	Joback Method
tc	897.59	K	Joback Method

Sources

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=U407149&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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