N-(2'-phenylethyl)propionamide

Inchi: InChI=1S/C11H15NO/c1-2-11(13)12-9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,13)
InchiKey: IABUULYQQIHCIL-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCC(O)=NCCc1ccccc1
Mol. weight [g/mol]: 177.24
CAS: 6283-04-1

Physical Properties

Property code	Value	Unit	Source
hf	-113.64	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.596		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
ripol	2587.00		NIST Webbook
tb	646.50	K	Joback Method
tc	854.33	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=C6283041&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature