

Propanamide, 3-phenyl-N-ethyl-

Inchi: InChI=1S/C11H15NO/c1-2-12-11(13)9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,13)
InchiKey: CUZZVRKUMNZZAY-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCN=C(O)CCc1ccccc1
Mol. weight [g/mol]: 177.24

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
rinpol	1663.00		NIST Webbook
tb	646.50	K	Joback Method
tc	854.33	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407147&Units=SI>
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>

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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