Phenylacetamide, N-butyl-

Inchi: InChI=1S/C12H17NO/c1-2-3-9-13-12(14)10-11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3,(H,1
InchiKey: JQZKYZUXIWDPAD-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCCCN=C(O)Cc1ccccc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
hf	-134.28	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.986		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	669.38	K	Joback Method
tc	874.28	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407223&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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