Phenylacetamide, N-isobutyl-

Inchi: InChI=1S/C12H17NO/c1-10(2)9-13-12(14)8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3,(H,1
InchiKey: CZMUPZDWASDNHR-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CC(C)CN=C(O)Cc1ccccc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
hf	-139.56	kJ/mol	Joback Method
hvap	64.27	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.842		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	668.94	K	Joback Method
tc	877.55	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407222&Units=SI

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