Isobutylcarbamate, N-benzyl

Inchi: InChI=1S/C12H17NO2/c1-10(2)9-15-12(14)13-8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3,

InchiKey: LTJFRJHNUIOOST-UHFFFAOYSA-N

Formula: C12H17NO2

SMILES: CC(C)COC(O)=NCc1ccccc1

Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
hf	-271.78	kJ/mol	Joback Method
hvap	66.68	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.773		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	691.36	K	Joback Method
tc	898.05	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R392548&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

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