Benzamide, 3-methyl-N-butyl-

Inchi: InChI=1S/C12H17NO/c1-3-4-8-13-12(14)11-7-5-6-10(2)9-11/h5-7,9H,3-4,8H2,1-2H3,(H,1

InchiKey: NXDWJMPJVGIQBB-UHFFFAOYSA-N

Formula: C12H17NO

SMILES: CCCCN=C(O)c1cccc(C)c1

Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
hf	-145.75	kJ/mol	Joback Method
hvap	65.32	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	3.100		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1766.00		NIST Webbook
tb	674.36	K	Joback Method
tc	880.11	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407411&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