Benzamide, 2-methyl-N-(3-methylbutyl)-

Inchi: InChI=1S/C13H19NO/c1-10(2)8-9-14-13(15)12-7-5-4-6-11(12)3/h4-7,10H,8-9H2,1-3H3,(
InchiKey: YNDNHEOIDGCSOS-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: Cc1ccccc1C(O)=NCCC(C)C
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
hf	-171.67	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.346		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	696.80	K	Joback Method
tc	903.40	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407395&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