Benzamide, 3-bromo-N-(3-methylbutyl)-

Inchi: InChI=1S/C12H16BrNO/c1-9(2)6-7-14-12(15)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H
InchiKey: IKJZQBZKPJUEJA-UHFFFAOYSA-N
Formula: C12H16BrNO
SMILES: CC(C)CCN=C(O)c1cccc(Br)c1
Mol. weight [g/mol]: 270.17

Physical Properties

Property code	Value	Unit	Source
hf	-124.70	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.800		Crippen Method
mcvol	185.230	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	2016.00		NIST Webbook
tb	740.08	K	Joback Method
tc	959.94	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407205&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