Benzamide, 2-bromo-N-isobutyl-

Inchi: InChI=1S/C11H14BrNO/c1-8(2)7-13-11(14)9-5-3-4-6-10(9)12/h3-6,8H,7H2,1-2H3,(H,13,
InchiKey: UNFJEINMGBRHJZ-UHFFFAOYSA-N
Formula: C11H14BrNO
SMILES: CC(C)CN=C(O)c1ccccc1Br
Mol. weight [g/mol]: 256.14

Physical Properties

Property code	Value	Unit	Source
hf	-104.06	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.410		Crippen Method
mcvol	171.140	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	717.20	K	Joback Method
tc	940.57	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407113&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