Benzamide, 2-bromo-N-butyl-

Inchi: InChI=1S/C11H14BrNO/c1-2-3-8-13-11(14)9-6-4-5-7-10(9)12/h4-7H,2-3,8H2,1H3,(H,13,
InchiKey: PVEIQVRGXQHPBG-UHFFFAOYSA-N
Formula: C11H14BrNO
SMILES: CCCCN=C(O)c1ccccc1Br
Mol. weight [g/mol]: 256.14

Physical Properties

Property code	Value	Unit	Source
hf	-98.78	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.554		Crippen Method
mcvol	171.140	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	717.64	K	Joback Method
tc	937.03	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407114&Units=SI

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