Benzamide, 2-bromo-N-methyl-

Inchi:	InChI=1S/C8H8BrNO/c1-10-8(11)6-4-2-3-5-7(6)9/h2-5H,1H3,(H,10,11)
InchiKey:	FKVCJQNPXXXZIE-UHFFFAOYSA-N
Formula:	C8H8BrNO
SMILES:	CN=C(O)c1ccccc1Br
Mol. weight [g/mol]:	214.06

Physical Properties

Property code	Value	Unit	Source
hf	-36.86	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.384		Crippen Method
mcvol	128.870	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
tb	649.00	K	Joback Method
tc	880.53	K	Joback Method

Sources

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=U407111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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