

# Benzamide, 3-bromo-N-ethyl-

<b>Inchi:</b>	InChI=1S/C9H10BrNO/c1-2-11-9(12)7-4-3-5-8(10)6-7/h3-6H,2H2,1H3,(H,11,12)
<b>InchiKey:</b>	BYCKUGXGVHIJFY-UHFFFAOYSA-N
<b>Formula:</b>	C9H10BrNO
<b>SMILES:</b>	CCN=C(O)c1cccc(Br)c1
<b>Mol. weight [g/mol]:</b>	228.09

## Physical Properties

Property code	Value	Unit	Source
hf	-57.50	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.774		Crippen Method
mcvol	142.960	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	671.88	K	Joback Method
tc	898.99	K	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407201&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407201&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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