

# Benzamide, 3-bromo-N-(hept-2-yl)-

**Inchi:** InChI=1S/C14H20BrNO/c1-3-4-5-7-11(2)16-14(17)12-8-6-9-13(15)10-12/h6,8-11H,3-5,7H  
**InchiKey:** HUXCLRPTXAKIIZ-UHFFFAOYSA-N  
**Formula:** C14H20BrNO  
**SMILES:** CCCCCC(C)N=C(O)c1cccc(Br)c1  
**Mol. weight [g/mol]:** 298.22

## Physical Properties

Property code	Value	Unit	Source
hf	-165.98	kJ/mol	Joback Method
hvap	75.82	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.723		Crippen Method
mcvol	213.410	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	785.84	K	Joback Method
tc	1000.15	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407207&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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

<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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