

# Acetamide, N-(1-naphthyl)-2-bromo-

<b>Inchi:</b>	InChI=1S/C12H10BrNO/c13-8-12(15)14-11-7-3-5-9-4-1-2-6-10(9)11/h1-7H,8H2,(H,14,15)
<b>InchiKey:</b>	YTXQWCWHEKIEDH-UHFFFAOYSA-N
<b>Formula:</b>	C12H10BrNO
<b>SMILES:</b>	O=C(CBr)Nc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	264.12

## Physical Properties

Property code	Value	Unit	Source
gf	234.38	kJ/mol	Joback Method
hf	92.34	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.173		Crippen Method
mcvol	165.770	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinqol	2068.00		NIST Webbook
tb	694.80	K	Joback Method
tc	942.74	K	Joback Method
tf	459.03	K	Joback Method
vc	0.625	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.50	J/molxK	694.80	Joback Method
cpg	405.12	J/molxK	736.12	Joback Method
cpg	415.77	J/molxK	777.45	Joback Method
cpg	425.56	J/molxK	818.77	Joback Method
cpg	434.60	J/molxK	860.09	Joback Method
cpg	443.00	J/molxK	901.42	Joback Method
cpg	450.86	J/molxK	942.74	Joback Method

# Sources

<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>
<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=U307424&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307424&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion 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>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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