

# Bromoacetamide, N-ethyl-N-(3-methylphenyl)-

<b>Inchi:</b>	InChI=1S/C11H14BrNO/c1-3-13(11(14)8-12)10-6-4-5-9(2)7-10/h4-7H,3,8H2,1-2H3
<b>InchiKey:</b>	WWKAAGOKISIPBT-UHFFFAOYSA-N
<b>Formula:</b>	C11H14BrNO
<b>SMILES:</b>	CCN(C(=O)CBr)c1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	256.14

## Physical Properties

Property code	Value	Unit	Source
gf	140.70	kJ/mol	Joback Method
hf	-64.03	kJ/mol	Joback Method
hfus	27.80	kJ/mol	Joback Method
hvap	58.24	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.743		Crippen Method
mcvol	171.140	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	615.21	K	Joback Method
tc	837.60	K	Joback Method
tf	394.87	K	Joback Method
vc	0.629	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.83	J/mol×K	615.21	Joback Method
cpg	410.64	J/mol×K	652.27	Joback Method
cpg	423.49	J/mol×K	689.34	Joback Method
cpg	435.44	J/mol×K	726.40	Joback Method
cpg	446.56	J/mol×K	763.47	Joback Method
cpg	456.89	J/mol×K	800.53	Joback Method
cpg	466.49	J/mol×K	837.60	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=U308168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308168&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</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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