

# 5-Bromoacenaphthenone-2

<b>Inchi:</b>	InChI=1S/C12H7BrO/c13-10-5-4-9-11(14)6-7-2-1-3-8(10)12(7)9/h1-5H,6H2
<b>InchiKey:</b>	HFUWXIPPBJXMFN-UHFFFAOYSA-N
<b>Formula:</b>	C12H7BrO
<b>SMILES:</b>	O=C1Cc2cccc3c(Br)ccc1c23
<b>Mol. weight [g/mol]:</b>	247.09
<b>CAS:</b>	5386-09-4

## Physical Properties

Property code	Value	Unit	Source
gf	212.62	kJ/mol	Joback Method
hf	90.11	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	58.94	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.341		Crippen Method
mcvol	144.930	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	675.68	K	Joback Method
tc	944.36	K	Joback Method
tf	475.40	K	Joback Method
vc	0.556	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.39	J/molxK	675.68	Joback Method
cpg	343.73	J/molxK	720.46	Joback Method
cpg	354.17	J/molxK	765.24	Joback Method
cpg	363.85	J/molxK	810.02	Joback Method
cpg	372.91	J/molxK	854.80	Joback Method
cpg	381.46	J/molxK	899.58	Joback Method
cpg	389.64	J/molxK	944.36	Joback Method

# Sources

<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=C5386094&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5386094&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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