

# 2-Cyclohexenone,3-bromo,5,5-dimethyl-

<b>Other names:</b>	5,5-Dimethyl-3-bromocyclohex-2-enone 3-Bromo-5,5-dimethyl-cyclohex-2-enone
<b>Inchi:</b>	InChI=1S/C8H11BrO/c1-8(2)4-6(9)3-7(10)5-8/h3H,4-5H2,1-2H3
<b>InchiKey:</b>	LPZGJNIBSGPOED-UHFFFAOYSA-N
<b>Formula:</b>	C8H11BrO
<b>SMILES:</b>	CC1(C)CC(=O)C=C(Br)C1
<b>Mol. weight [g/mol]:</b>	203.08
<b>CAS:</b>	13271-49-3

## Physical Properties

Property code	Value	Unit	Source
gf	-52.50	kJ/mol	Joback Method
hf	-203.95	kJ/mol	Joback Method
hfus	7.64	kJ/mol	Joback Method
hvap	44.32	kJ/mol	Joback Method
ie	9.35	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.654		Crippen Method
mcvol	127.490	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	540.35	K	Joback Method
tc	791.23	K	Joback Method
tf	352.50	K	Joback Method
vc	0.469	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.93	J/molxK	540.35	Joback Method
cpg	285.19	J/molxK	582.16	Joback Method
cpg	298.53	J/molxK	623.98	Joback Method
cpg	311.08	J/molxK	665.79	Joback Method
cpg	322.97	J/molxK	707.60	Joback Method
cpg	334.32	J/molxK	749.42	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13271493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13271493&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>
<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>

## 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>ie:</b>	Ionization energy
<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>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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