

# 7a-Methyl-3-methylenehexahydrobenzofuran-2-one

<b>Inchi:</b>	InChI=1S/C10H14O2/c1-7-8-5-3-4-6-10(8,2)12-9(7)11/h8H,1,3-6H2,2H3
<b>InchiKey:</b>	CPAWXRWDKTXJD-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O2
<b>SMILES:</b>	C=C1C(=O)OC2(C)CCCC12
<b>Mol. weight [g/mol]:</b>	166.22
<b>CAS:</b>	67498-53-7

## Physical Properties

Property code	Value	Unit	Source
gf	-42.60	kJ/mol	Joback Method
hf	-292.83	kJ/mol	Joback Method
hfus	11.66	kJ/mol	Joback Method
hvap	45.96	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.048		Crippen Method
mvol	133.180	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1302.00		NIST Webbook
tb	548.66	K	Joback Method
tc	788.80	K	Joback Method
tf	360.15	K	Joback Method
vc	0.495	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.77	J/molxK	548.66	Joback Method
cpg	354.44	J/molxK	588.68	Joback Method
cpg	370.96	J/molxK	628.71	Joback Method
cpg	386.46	J/molxK	668.73	Joback Method
cpg	401.08	J/molxK	708.75	Joback Method
cpg	414.96	J/molxK	748.78	Joback Method
cpg	428.25	J/molxK	788.80	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C67498537&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C67498537&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>hvp:</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>rinp:</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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