

# (6R,7aR)-3,6-Dimethyl-5,6,7,7a-tetrahydrobenzofu

<b>Inchi:</b>	InChI=1S/C10H14O2/c1-6-3-4-8-7(2)10(11)12-9(8)5-6/h6,9H,3-5H2,1-2H3/t6-,9-/m1/s1
<b>InchiKey:</b>	VUVQBYIJRDUVHT-HZGVNTEJSA-N
<b>Formula:</b>	C10H14O2
<b>SMILES:</b>	CC1=C2CCC(C)CC2OC1=O
<b>Mol. weight [g/mol]:</b>	166.22
<b>CAS:</b>	38049-04-6

## Physical Properties

Property code	Value	Unit	Source
gf	-79.49	kJ/mol	Joback Method
hf	-357.47	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.048		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1499.70		NIST Webbook
tb	558.38	K	Joback Method
tc	791.07	K	Joback Method
tf	348.37	K	Joback Method
vc	0.499	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.43	J/molxK	558.38	Joback Method
cpg	355.83	J/molxK	597.16	Joback Method
cpg	372.24	J/molxK	635.94	Joback Method
cpg	387.67	J/molxK	674.73	Joback Method
cpg	402.16	J/molxK	713.51	Joback Method
cpg	415.71	J/molxK	752.29	Joback Method
cpg	428.34	J/molxK	791.07	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=C38049046&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38049046&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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