

# 1-Isopropyl-4-methyl-7-oxa-bicyclo[4.1.0]heptane

<b>Inchi:</b>	InChI=1S/C10H18O/c1-7(2)10-5-4-8(3)6-9(10)11-10/h7-9H,4-6H2,1-3H3
<b>InchiKey:</b>	PPERHRAPFJGBED-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O
<b>SMILES:</b>	CC1CCC2(C(C)C)OC2C1
<b>Mol. weight [g/mol]:</b>	154.25
<b>CAS:</b>	4184-02-5

## Physical Properties

Property code	Value	Unit	Source
chl	-5450.90	kJ/mol	NIST Webbook
gf	40.96	kJ/mol	Joback Method
hf	-252.67	kJ/mol	Joback Method
hfus	15.05	kJ/mol	Joback Method
hvap	40.51	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.600		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	468.03	K	Joback Method
tc	677.82	K	Joback Method
tf	266.05	K	Joback Method
vc	0.513	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.17	J/molxK	468.03	Joback Method
cpg	340.52	J/molxK	502.99	Joback Method
cpg	358.49	J/molxK	537.96	Joback Method
cpg	375.19	J/molxK	572.92	Joback Method
cpg	390.78	J/molxK	607.89	Joback Method
cpg	405.39	J/molxK	642.85	Joback Method
cpg	419.16	J/molxK	677.82	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=C4184025&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4184025&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>mconvol:</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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