

# (3aR,4S,7R,7aS)-3a,7a-Dimethyloctahydro-1H-4,7-

<b>Inchi:</b>	InChI=1S/C12H20/c1-11-6-3-7-12(11,2)10-5-4-9(11)8-10/h9-10H,3-8H2,1-2H3
<b>InchiKey:</b>	ZHFYGOWNPVBAAC-UHFFFAOYSA-N
<b>Formula:</b>	C12H20
<b>SMILES:</b>	CC12CCCC1(C)C1CCC2C1
<b>Mol. weight [g/mol]:</b>	164.29
<b>CAS:</b>	67152-02-7

## Physical Properties

Property code	Value	Unit	Source
gf	201.62	kJ/mol	Joback Method
hf	-68.63	kJ/mol	Joback Method
hfus	7.62	kJ/mol	Joback Method
hvap	39.61	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.613		Crippen Method
mvol	147.360	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1199.10		NIST Webbook
tb	494.26	K	Joback Method
tc	720.37	K	Joback Method
tf	318.86	K	Joback Method
vc	0.566	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.32	J/molxK	494.26	Joback Method
cpg	390.80	J/molxK	531.94	Joback Method
cpg	411.27	J/molxK	569.63	Joback Method
cpg	430.04	J/molxK	607.31	Joback Method
cpg	447.41	J/molxK	645.00	Joback Method
cpg	463.70	J/molxK	682.68	Joback Method
cpg	479.22	J/molxK	720.37	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C67152027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C67152027&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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