

# 1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-, (1«alpha»,3a«alpha»,4«beta»,7«alpha»,8a«beta»)-

Other names: Isopatchoulane  
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-

**Inchi:** InChI=1S/C15H26/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h10-13H,5-9H2,1-4H3

**InchiKey:** MVZZUMCHPFHUOS-UHFFFAOYSA-N

**Formula:** C15H26

**SMILES:** CC1CCC23C(C)CCC(CC12)C3(C)C

**Mol. weight [g/mol]:** 206.37

**CAS:** 3724-42-3

## Physical Properties

Property code	Value	Unit	Source
gf	199.36	kJ/mol	Joback Method
hf	-177.39	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.495		Crippen Method
mvol	189.630	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1552.00		NIST Webbook
tb	557.83	K	Joback Method
tc	780.06	K	Joback Method
tf	340.67	K	Joback Method
vc	0.724	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/molxK	557.83	Joback Method
cpg	547.59	J/molxK	594.87	Joback Method
cpg	570.94	J/molxK	631.91	Joback Method
cpg	592.86	J/molxK	668.95	Joback Method
cpg	613.64	J/molxK	705.99	Joback Method
cpg	633.54	J/molxK	743.02	Joback Method

## Sources

<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=C3724423&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3724423&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>mcpvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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