

# 4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-, [1S-(1«alpha»,4«alpha»,7«alpha»)]-

Other names: «beta» Patchoulene  
(1S,4S,7R)-1,4,9,9-Tetramethyl-1,2,3,4,5,6,7,8-octahydro-4,7-methanoazulene

4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-  
[1S-(1 «alpha»,4 «alpha»,7 «alpha»)]-1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-4,7-methanoazulene

**Inchi:** InChI=1S/C15H24/c1-10-5-6-13-12(10)9-11-7-8-15(13,4)14(11,2)3/h10-11H,5-9H2,1-4H3

**InchiKey:** CSKINCSXMLCMAR-UEKVPHQBSA-N

**Formula:** C15H24

**SMILES:** CC1CCC2=C1CC1CCC2(C)C1(C)C

**Mol. weight [g/mol]:** 204.35

**CAS:** 514-51-2

## Physical Properties

Property code	Value	Unit	Source
gf	225.48	kJ/mol	Joback Method
hf	-101.87	kJ/mol	Joback Method
hfus	13.73	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1378.00		NIST Webbook

rinpol	1385.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	576.29	K	Joback Method
tc	802.89	K	Joback Method
tf	374.95	K	Joback Method
vc	0.712	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.46	J/molxK	576.29	Joback Method
cpg	525.54	J/molxK	614.06	Joback Method
cpg	546.15	J/molxK	651.82	Joback Method

cpg	565.60	J/mol×K	689.59	Joback Method
cpg	584.18	J/mol×K	727.36	Joback Method
cpg	602.19	J/mol×K	765.12	Joback Method
cpg	619.93	J/mol×K	802.89	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C514512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C514512&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.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>

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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