

# 1,2,4a,9-Tetramethyl-1,2,3,4,4a,5,6,14b-octahydro-

<b>Inchi:</b>	InChI=1S/C26H30/c1-16-12-14-26(4)15-13-23-22-9-8-19-17(2)6-5-7-20(19)21(22)10-11-
<b>InchiKey:</b>	DDHCCKRACZWQKU-UHFFFAOYSA-N
<b>Formula:</b>	C26H30
<b>SMILES:</b>	<chem>Cc1cccc2c1ccc1c3c(ccc12)C1C(C)C(C)CCC1(C)CC3</chem>
<b>Mol. weight [g/mol]:</b>	342.52

## Physical Properties

Property code	Value	Unit	Source
gf	531.62	kJ/mol	Joback Method
hf	100.66	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	80.07	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	7.404		Crippen Method
mcvol	292.800	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	3099.27		NIST Webbook
tb	891.76	K	Joback Method
tc	1141.03	K	Joback Method
tf	568.94	K	Joback Method
vc	1.121	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.78	J/molxK	891.76	Joback Method
cpg	993.79	J/molxK	933.31	Joback Method
cpg	1017.63	J/molxK	974.85	Joback Method
cpg	1041.63	J/molxK	1016.40	Joback Method
cpg	1066.12	J/molxK	1057.94	Joback Method
cpg	1091.43	J/molxK	1099.49	Joback Method
cpg	1117.88	J/molxK	1141.03	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=R179672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R179672&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>

# 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>h vap:</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>m cvol:</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

Latest version available from:

<https://www.chemeo.com/cid/23-423-6/1-2-4a-9-Tetramethyl-1-2-3-4-4a-5-6-14b-octahydro-picene.pdf>

Generated by Cheméo on 2024-04-26 04:34:57.30944917 +0000 UTC m=+16395346.230026482.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.