

# Perhydrophenanthrene, 2B,4bB,8,8,10aB-pentamethyl-1A-(3S-methyl-7-ox

Inchi:	InChI=1S/C28H50O/c1-20(10-8-11-22(3)29)12-14-23-21(2)13-15-25-27(23,6)19-16-24-2
InchiKey:	DJTIKPPBMWKDMJ-MMFNPOGVSA-N
Formula:	C28H50O
SMILES:	CC(=O)CCCC(C)CCC1C(C)CCC2C1(C)CCC1C(C)(C)CCCC12C
Mol. weight [g/mol]:	402.70

## Physical Properties

Property code	Value	Unit	Source
gf	127.96	kJ/mol	Joback Method
hf	-587.15	kJ/mol	Joback Method
hfus	35.65	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	8.457		Crippen Method
mcvol	374.370	ml/mol	McGowan Method
pc	908.89	kPa	Joback Method
rinsol	3050.00		NIST Webbook
tb	917.08	K	Joback Method
tc	1137.68	K	Joback Method
tf	531.21	K	Joback Method
vc	1.425	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1372.45	J/molxK	917.08	Joback Method
cpg	1406.44	J/molxK	953.85	Joback Method
cpg	1441.15	J/molxK	990.61	Joback Method
cpg	1476.94	J/molxK	1027.38	Joback Method
cpg	1514.20	J/molxK	1064.15	Joback Method
cpg	1553.28	J/molxK	1100.92	Joback Method
cpg	1594.57	J/molxK	1137.68	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=R556955&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R556955&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>

# 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>hvac:</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>mccol:</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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