

# Perhydrophenanthrene, 2A,4bB,8,8,10aB-pentamethyl-1A-(3-oxobutyl)

Inchi:	InChI=1S/C23H40O/c1-16-8-11-20-22(5,18(16)10-9-17(2)24)15-12-19-21(3,4)13-7-14-23
InchiKey:	XNAGUWARFHSTGQ-MYRYCMPCSA-N
Formula:	C23H40O
SMILES:	CC(=O)CCC1C(C)CCC2C1(C)CCC1C(C)(C)CCCC12C
Mol. weight [g/mol]:	332.56

## Physical Properties

Property code	Value	Unit	Source
gf	88.30	kJ/mol	Joback Method
hf	-478.67	kJ/mol	Joback Method
hfus	26.22	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.651		Crippen Method
mvol	303.920	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	803.12	K	Joback Method
tc	1029.06	K	Joback Method
tf	489.86	K	Joback Method
vc	1.151	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.58	J/molxK	803.12	Joback Method
cpg	1063.94	J/molxK	840.78	Joback Method
cpg	1093.22	J/molxK	878.43	Joback Method
cpg	1122.79	J/molxK	916.09	Joback Method
cpg	1153.04	J/molxK	953.75	Joback Method
cpg	1184.34	J/molxK	991.40	Joback Method
cpg	1217.07	J/molxK	1029.06	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=R556900&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R556900&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>rinpola:</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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