

# (1As-(1a«alpha»,4b«beta»,8as)-4a,8,8-trimethyloc

<b>Other names:</b>	(1aS,4aR,8aR)-4a,8,8-Trimethyloctahydrocyclopropa[d]naphthalen-2(3H)-one
<b>Inchi:</b>	InChI=1S/C14H22O/c1-12(2)6-4-7-13(3)8-5-11(15)10-9-14(10,12)13/h10H,4-9H2,1-3H3
<b>InchiKey:</b>	OZVBAFBRWKCHV-UHFFFAOYSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC1(C)CCCC2(C)CCC(=O)C3CC312
<b>Mol. weight [g/mol]:</b>	206.32
<b>CAS:</b>	82262-79-1

## Physical Properties

Property code	Value	Unit	Source
gf	78.28	kJ/mol	Joback Method
hf	-238.53	kJ/mol	Joback Method
hfus	3.91	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.572		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1723.10		NIST Webbook
rinpol	1723.10		NIST Webbook
tb	612.35	K	Joback Method
tc	862.61	K	Joback Method
tf	430.00	K	Joback Method
vc	0.674	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.56	J/molxK	612.35	Joback Method
cpg	529.66	J/molxK	654.06	Joback Method
cpg	550.53	J/molxK	695.77	Joback Method
cpg	570.66	J/molxK	737.48	Joback Method
cpg	590.55	J/molxK	779.19	Joback Method
cpg	610.71	J/molxK	820.90	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C82262791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82262791&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>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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