

# 12-O-Methylcarnosol

<b>Inchi:</b>	InChI=1S/C21H28O4/c1-11(2)12-9-13-14-10-15-20(3,4)7-6-8-21(15,19(23)25-14)16(13)1
<b>InchiKey:</b>	SLKLTJLWMEJLZ-UHFFFAOYSA-N
<b>Formula:</b>	C21H28O4
<b>SMILES:</b>	COc1c(C(C)C)cc2c(c1O)C13CCCC(C)(C)C1CC2OC3=O
<b>Mol. weight [g/mol]:</b>	344.44
<b>CAS:</b>	85514-27-8

## Physical Properties

Property code	Value	Unit	Source
gf	-109.85	kJ/mol	Joback Method
hf	-636.78	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.590		Crippen Method
mcvol	269.590	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	2831.20		NIST Webbook
rinpol	2831.20		NIST Webbook
tb	939.17	K	Joback Method
tc	1189.01	K	Joback Method
tf	698.01	K	Joback Method
vc	0.968	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.37	J/molxK	939.17	Joback Method
cpg	984.53	J/molxK	980.81	Joback Method
cpg	1013.15	J/molxK	1022.45	Joback Method
cpg	1043.67	J/molxK	1064.09	Joback Method
cpg	1076.51	J/molxK	1105.73	Joback Method
cpg	1112.10	J/molxK	1147.37	Joback Method
cpg	1150.86	J/molxK	1189.01	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C85514278&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85514278&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>

# 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>hvp:</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>rinp:</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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