

# Desoxyhumulone

**Inchi:** InChI=1S/C21H30O4/c1-12(2)7-9-15-19(23)16(10-8-13(3)4)21(25)18(20(15)24)17(22)11  
**InchiKey:** NQYBQBZOHCACCR-UHFFFAOYSA-N  
**Formula:** C21H30O4  
**SMILES:** CC(C)=CCc1c(O)c(CC=C(C)C)c(O)c(C(=O)CC(C)C)c1O  
**Mol. weight [g/mol]:** 346.46

## Physical Properties

Property code	Value	Unit	Source
gf	-232.79	kJ/mol	Joback Method
hf	-698.11	kJ/mol	Joback Method
hfus	56.62	kJ/mol	Joback Method
hvap	111.42	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.050		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	1019.89	K	Joback Method
tc	1258.44	K	Joback Method
tf	709.90	K	Joback Method
vc	0.964	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.40	J/mol×K	1019.89	Joback Method
cpg	1004.24	J/mol×K	1059.65	Joback Method
cpg	1025.99	J/mol×K	1099.41	Joback Method
cpg	1048.94	J/mol×K	1139.17	Joback Method
cpg	1073.34	J/mol×K	1178.93	Joback Method
cpg	1099.45	J/mol×K	1218.68	Joback Method
cpg	1127.55	J/mol×K	1258.44	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=R97054&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R97054&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>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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