

# Tetrahydrocannabinol

<b>Inchi:</b>	InChI=1S/C21H30O2/c1-5-6-7-8-15-12-18(22)20-16-11-14(2)9-10-17(16)21(3,4)23-19(20)
<b>InchiKey:</b>	SJQJFSCMYCROHP-UHFFFAOYSA-N
<b>Formula:</b>	C21H30O2
<b>SMILES:</b>	CCCCC1CC2=C(c3cc(C)ccc3C(C)(C)O2)C(O)C1
<b>Mol. weight [g/mol]:</b>	314.46
<b>CAS:</b>	56282-24-7

## Physical Properties

Property code	Value	Unit	Source
gf	90.95	kJ/mol	Joback Method
hf	-384.39	kJ/mol	Joback Method
hfus	42.76	kJ/mol	Joback Method
hvap	87.45	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.323		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2452.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2490.00		NIST Webbook
tb	862.36	K	Joback Method
tc	1075.33	K	Joback Method
tf	539.58	K	Joback Method
vc	1.024	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.36	J/mol×K	862.36	Joback Method
cpg	902.49	J/mol×K	897.86	Joback Method
cpg	921.24	J/mol×K	933.35	Joback Method
cpg	939.77	J/mol×K	968.85	Joback Method
cpg	958.22	J/mol×K	1004.34	Joback Method
cpg	976.76	J/mol×K	1039.84	Joback Method
cpg	995.53	J/mol×K	1075.33	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C56282247&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56282247&amp;Units=SI</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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