

# Taraxastane (19-«beta»-H)

**Inchi:** InChI=1S/C30H52/c1-20-12-16-27(5)18-19-29(7)22(25(27)21(20)2)10-11-24-28(6)15-9-1  
**InchiKey:** OOTXFYSZXCMPG-BDUQRCOBSA-N  
**Formula:** C30H52  
**SMILES:** CC1CCC2(C)CCC3(C)C(CCC4C5(C)CCCC(C)(C)C5CCC43C)C2C1C  
**Mol. weight [g/mol]:** 412.73

## Physical Properties

Property code	Value	Unit	Source
gf	347.06	kJ/mol	Joback Method
hf	-387.49	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	9.134		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	3388.00		NIST Webbook
tb	922.57	K	Joback Method
tc	1168.67	K	Joback Method
tf	586.98	K	Joback Method
vc	1.429	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.19	J/mol×K	922.57	Joback Method
cpg	1509.87	J/mol×K	963.59	Joback Method
cpg	1560.69	J/mol×K	1004.60	Joback Method
cpg	1615.46	J/mol×K	1045.62	Joback Method
cpg	1674.98	J/mol×K	1086.64	Joback Method
cpg	1740.07	J/mol×K	1127.66	Joback Method
cpg	1811.54	J/mol×K	1168.67	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=R215604&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R215604&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>hvac:</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>mccol:</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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