

# «beta»-Microbiotene

<b>Inchi:</b>	InChI=1S/C15H24/c1-11-6-9-15(10-12(11)15)14(4)8-5-7-13(14,2)3/h12H,1,5-10H2,2-4H3
<b>InchiKey:</b>	YMPBLULPBSVQLP-SNPRPXQ TSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C1CCC2(C3(C)CCCC3(C)C)CC12</chem>
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	262.37	kJ/mol	Joback Method
hf	-37.23	kJ/mol	Joback Method
hfus	5.83	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mvol	185.330	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	566.57	K	Joback Method
tc	800.20	K	Joback Method
tf	386.73	K	Joback Method
vc	0.708	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.14	J/mol×K	566.57	Joback Method
cpg	522.76	J/mol×K	605.51	Joback Method
cpg	543.69	J/mol×K	644.45	Joback Method
cpg	563.39	J/mol×K	683.38	Joback Method
cpg	582.28	J/mol×K	722.32	Joback Method
cpg	600.82	J/mol×K	761.26	Joback Method
cpg	619.44	J/mol×K	800.20	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=R620794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R620794&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>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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