

# «beta»-Cyclocostunolide

<b>Inchi:</b>	InChI=1S/C15H20O2/c1-9-5-4-7-15(3)8-6-11-10(2)14(16)17-13(11)12(9)15/h11-13H,1-2,
<b>InchiKey:</b>	XUYAKPXYKQEFPD-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O2
<b>SMILES:</b>	<chem>C=C1C(=O)OC2C1CCC1(C)CCCC(=C)C21</chem>
<b>Mol. weight [g/mol]:</b>	232.32
<b>CAS:</b>	2221-82-1

## Physical Properties

Property code	Value	Unit	Source
gf	93.52	kJ/mol	Joback Method
hf	-265.49	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	57.03	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.241		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1983.40		NIST Webbook
rinpol	1983.40		NIST Webbook
tb	668.56	K	Joback Method
tc	911.16	K	Joback Method
tf	440.36	K	Joback Method
vc	0.708	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.67	J/mol×K	668.56	Joback Method
cpg	580.06	J/mol×K	708.99	Joback Method
cpg	600.23	J/mol×K	749.43	Joback Method
cpg	619.34	J/mol×K	789.86	Joback Method
cpg	637.56	J/mol×K	830.29	Joback Method
cpg	655.08	J/mol×K	870.73	Joback Method
cpg	672.06	J/mol×K	911.16	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C2221821&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2221821&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>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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