

# 31-Norcycloartenol acetate

<b>Inchi:</b>	InChI=1S/C31H50O2/c1-20(2)9-8-10-21(3)23-11-12-24-25-13-14-26-28(5,6)27(33-22(4)3
<b>InchiKey:</b>	JAWKBSRSXOOGCI-HFCUEOPBSA-N
<b>Formula:</b>	C31H50O2
<b>SMILES:</b>	CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCC=C(C)C)CCC2C4CCC3C1(C)C
<b>Mol. weight [g/mol]:</b>	454.73

## Physical Properties

Property code	Value	Unit	Source
gf	260.10	kJ/mol	Joback Method
hf	-500.70	kJ/mol	Joback Method
hfus	37.67	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.350		Crippen Method
mcvol	396.490	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpola	3321.00		NIST Webbook
tb	1017.36	K	Joback Method
tc	1255.97	K	Joback Method
tf	635.03	K	Joback Method
vc	1.520	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.47	J/molxK	1017.36	Joback Method
cpg	1626.31	J/molxK	1057.13	Joback Method
cpg	1680.28	J/molxK	1096.90	Joback Method
cpg	1739.07	J/molxK	1136.67	Joback Method
cpg	1803.38	J/molxK	1176.44	Joback Method
cpg	1873.88	J/molxK	1216.21	Joback Method
cpg	1951.28	J/molxK	1255.97	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=R110668&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R110668&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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