

# Cyclobranol (24-methylcycloartenol) acetate

<b>Inchi:</b>	InChI=1S/C33H54O2/c1-21(2)22(3)10-11-23(4)25-14-16-31(9)27-13-12-26-29(6,7)28(35)
<b>InchiKey:</b>	QADDYABFNQGSOG-KGTVBQRLSA-N
<b>Formula:</b>	C33H54O2
<b>SMILES:</b>	CC(=O)OC1CCC23CC24CCC2(C)C(C(C)CCC(C)=C(C)C)CCC2(C)C4CCC3C1(C)C
<b>Mol. weight [g/mol]:</b>	482.78

## Physical Properties

Property code	Value	Unit	Source
gf	262.90	kJ/mol	Joback Method
hf	-536.53	kJ/mol	Joback Method
hfus	35.24	kJ/mol	Joback Method
hvap	91.03	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	9.130		Crippen Method
mcvol	424.670	ml/mol	McGowan Method
pc	839.19	kPa	Joback Method
rinsol	3498.00		NIST Webbook
tb	1063.24	K	Joback Method
tc	1308.14	K	Joback Method
tf	667.51	K	Joback Method
vc	1.631	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.39	J/molxK	1063.24	Joback Method
cpg	1821.83	J/molxK	1104.06	Joback Method
cpg	1893.89	J/molxK	1144.87	Joback Method
cpg	1973.48	J/molxK	1185.69	Joback Method
cpg	2061.46	J/molxK	1226.51	Joback Method
cpg	2158.70	J/molxK	1267.32	Joback Method
cpg	2266.10	J/molxK	1308.14	Joback Method

# Sources

<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=R111087&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R111087&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>mccvol:</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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