

# Secoandrost-5-ene-16-peroxyacetic acid, 16,17-,17-carboxy-3-beta-hydroxy-,

Inchi: CCOC(=O)C1(C)CCC2C(CC=C3CC(OC(C)=O)CCC32C)C1CC(=O)OOC(C)(C)C  
InchiKey: IKTQPPCFEIUQLK-JHFFFAOYSA-N

Formula: C<sub>26</sub>H<sub>40</sub>O<sub>7</sub>

SMILES: COC(=O)C1(C)CCC2C(CC=C3CC(OC(C)=O)CCC32C)C1CC(=O)OOC(C)(C)C

Mol. weight [g/mol]: 464.59

## Physical Properties

Property code	Value	Unit	Source
gf	-527.91	kJ/mol	Joback Method
hf	-1251.97	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	100.38	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.924		Crippen Method
mcvol	368.510	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
tb	1074.52	K	Joback Method
tc	1317.76	K	Joback Method
tf	708.49	K	Joback Method
vc	1.381	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1405.83	J/molxK	1074.52	Joback Method
cpg	1435.89	J/molxK	1115.06	Joback Method
cpg	1466.75	J/molxK	1155.60	Joback Method
cpg	1498.71	J/molxK	1196.14	Joback Method
cpg	1532.08	J/molxK	1236.68	Joback Method
cpg	1567.15	J/molxK	1277.22	Joback Method
cpg	1604.24	J/molxK	1317.76	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005264&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005264&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>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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