

# «beta»-Eudesmol, acetate

<b>Inchi:</b>	InChI=1S/C17H28O2/c1-12-7-6-9-17(5)10-8-14(11-15(12)17)16(3,4)19-13(2)18/h14-15H
<b>InchiKey:</b>	UIMWPYYFYGCEJP-AYWPPYMVSA-N
<b>Formula:</b>	C17H28O2
<b>SMILES:</b>	C=C1CCCC2(C)CCC(C(C)(C)OC(C)=O)CC12
<b>Mol. weight [g/mol]:</b>	264.40

## Physical Properties

Property code	Value	Unit	Source
gf	-25.84	kJ/mol	Joback Method
hf	-447.66	kJ/mol	Joback Method
hfus	16.64	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.491		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1793.00		NIST Webbook
rinpol	1791.70		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	686.71	K	Joback Method
tc	910.63	K	Joback Method
tf	411.07	K	Joback Method
vc	0.864	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.66	J/mol×K	686.71	Joback Method
cpg	715.30	J/mol×K	724.03	Joback Method

cpg	736.67	J/mol×K	761.35	Joback Method
cpg	756.94	J/mol×K	798.67	Joback Method
cpg	776.26	J/mol×K	835.99	Joback Method
cpg	794.79	J/mol×K	873.31	Joback Method
cpg	812.70	J/mol×K	910.63	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=R129761&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R129761&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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