

# Ergosta-5,22-dien-3-ol, acetate, (3«beta»,22E)-

<b>Other names:</b>	Brassicasterol acetate
<b>Inchi:</b>	InChI=1S/C30H48O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31
<b>InchiKey:</b>	YAXRKAKOIWXVHL-CMDGGOBGSA-N
<b>Formula:</b>	C30H48O2
<b>SMILES:</b>	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)C=CC(C)C(C)C)CCC32)C1
<b>Mol. weight [g/mol]:</b>	440.70
<b>CAS:</b>	2458-53-9

## Physical Properties

Property code	Value	Unit	Source
gf	209.42	kJ/mol	Joback Method
hf	-529.78	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.982		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	3224.00		NIST Webbook
tb	1003.85	K	Joback Method
tc	1239.22	K	Joback Method
tf	552.46	K	Joback Method
vc	1.468	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.08	J/molxK	1003.85	Joback Method
cpg	1511.34	J/molxK	1043.08	Joback Method
cpg	1546.51	J/molxK	1082.31	Joback Method
cpg	1582.99	J/molxK	1121.54	Joback Method
cpg	1621.14	J/molxK	1160.76	Joback Method
cpg	1661.37	J/molxK	1199.99	Joback Method
cpg	1704.06	J/molxK	1239.22	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=C2458539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2458539&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>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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