

# Isobauerenol (8-bauerenol) acetate

<b>Inchi:</b>	InChI=1S/C32H52O2/c1-20-12-15-29(6)18-19-31(8)24-10-11-25-28(4,5)26(34-22(3)33)1
<b>InchiKey:</b>	GXGXUGKOSZFXNS-XKRMTFNLSA-N
<b>Formula:</b>	C32H52O2
<b>SMILES:</b>	CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC2(C)CCC(C)C(C)C2C1(C)CC3
<b>Mol. weight [g/mol]:</b>	468.75

## Physical Properties

Property code	Value	Unit	Source
gf	148.39	kJ/mol	Joback Method
hf	-618.39	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.740		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	889.47	kPa	Joback Method
rinqol	3387.00		NIST Webbook
tb	1058.41	K	Joback Method
tc	1308.83	K	Joback Method
tf	711.72	K	Joback Method
vc	1.552	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1700.06	J/molxK	1058.41	Joback Method
cpg	1762.02	J/molxK	1100.15	Joback Method
cpg	1829.75	J/molxK	1141.88	Joback Method
cpg	1904.08	J/molxK	1183.62	Joback Method
cpg	1985.83	J/molxK	1225.36	Joback Method
cpg	2075.84	J/molxK	1267.09	Joback Method
cpg	2174.92	J/molxK	1308.83	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=R111285&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R111285&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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