

# [14C] GA25 16«alpha», 17-H2, 17-OH , methyl ester

Inchi:	InChI=1S/C23H34O6/c1-13-11-22-12-14(13)7-8-15(22)23(20(26)29-5)10-6-9-21(2,19(25
InchiKey:	UXXGYXYHILQJBU-UMFNCLRBSA-N
Formula:	C23H34O6
SMILES:	COC(=O)C1C2C(C)(C(=O)OC)CCCC2(C(=O)OC)C2CCC3CC12CC3C
Mol. weight [g/mol]:	406.51

## Physical Properties

Property code	Value	Unit	Source
gf	-399.59	kJ/mol	Joback Method
hf	-1015.37	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	89.74	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.370		Crippen Method
mcvol	313.810	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	976.32	K	Joback Method
tc	1211.33	K	Joback Method
tf	681.39	K	Joback Method
vc	1.190	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.09	J/molxK	976.32	Joback Method
cpg	1214.32	J/molxK	1015.49	Joback Method
cpg	1248.32	J/molxK	1054.66	Joback Method
cpg	1284.51	J/molxK	1093.82	Joback Method
cpg	1323.30	J/molxK	1132.99	Joback Method
cpg	1365.12	J/molxK	1172.16	Joback Method
cpg	1410.38	J/molxK	1211.33	Joback Method

# Sources

<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=R190857&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R190857&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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