# [14C] GA15, methyl ester

**Inchi:** InChI=1S/C21H28O4/c1-12-9-21-10-13(12)5-6-14(21)20-8-4-7-19(2,18(23)25-11-20)16(2
**InchiKey:** SDNANUVFTHNCBP-QNUBZUTLSA-N
**Formula:** C21H28O4
**SMILES:** C=C1CC23CC1CCC2C12CCCC(C)(C(=O)OC1)C2C3C(=O)OC
**Mol. weight [g/mol]:** 344.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -28.05 | kJ/mol | Joback Method |
| hf | -556.47 | kJ/mol | Joback Method |
| hfus | 26.89 | kJ/mol | Joback Method |
| hvap | 76.42 | kJ/mol | Joback Method |
| log10ws | -3.97 | | Crippen Method |
| logp | 3.501 | | Crippen Method |
| mcvol | 263.030 | ml/mol | McGowan Method |
| pc | 1812.32 | kPa | Joback Method |
| rinpol | 2594.00 | | NIST Webbook |
| rinpol | 2588.00 | | NIST Webbook |
| rinpol | 2594.00 | | NIST Webbook |
| rinpol | 2594.00 | | NIST Webbook |
| rinpol | 2587.00 | | NIST Webbook |
| tb | 887.99 | K | Joback Method |
| tc | 1139.83 | K | Joback Method |
| tf | 649.42 | K | Joback Method |
| vc | 1.000 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 954.19 | J/mol×K | 887.99 | Joback Method |
| cpg | 983.54 | J/mol×K | 929.96 | Joback Method |
| cpg | 1014.48 | J/mol×K | 971.94 | Joback Method |
| cpg | 1047.57 | J/mol×K | 1013.91 | Joback Method |
| cpg | 1083.38 | J/mol×K | 1055.88 | Joback Method |

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|---|---|---|---|---|
| cpg | 1122.47 | J/mol×K | 1097.86 | Joback Method |
| cpg | 1165.40 | J/mol×K | 1139.83 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R190802&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |