[14C] GA15-15,16-ene methyl ester

Other names: GA15-15,16-ene 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: JTJQFHFZNVWSPQ-QNUBZUTLSA-N
Formula: C21H28O4
SMILES: COC(=O)C1C2C3(C)CCCC2(COC3=O)C2CCC3CC12C=C3C
Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-60.80	kJ/mol	Joback Method
hf	-594.40	kJ/mol	Joback Method
hfus	28.88	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.501		Crippen Method
mcvol	263.030	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	892.97	K	Joback Method
tc	1145.65	K	Joback Method
tf	649.02	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.10	J/mol×K	892.97	Joback Method
cpg	984.71	J/mol×K	935.08	Joback Method
cpg	1016.03	J/mol×K	977.20	Joback Method
cpg	1049.63	J/mol×K	1019.31	Joback Method
cpg	1086.08	J/mol×K	1061.43	Joback Method
cpg	1125.96	J/mol×K	1103.54	Joback Method
cpg	1169.83	J/mol×K	1145.65	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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