[14C4]GA24 methyl ester

Inchi: InChI=1S/C22H30O5/c1-13-10-22-11-14(13)6-7-15(22)21(12-23)9-5-8-20(2,19(25)27-4)1
InchiKey: CDZKHHKZGGMPOC-RTOKLNTCSA-N
Formula: C22H30O5
SMILES: C=C1CC23CC1CCC2C1(C=O)CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 374.47

Physical Properties

Property code	Value	Unit	Source
gf	-212.82	kJ/mol	Joback Method
hf	-730.93	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.317		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook
tb	929.64	K	Joback Method
tc	1164.39	K	Joback Method
tf	657.88	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.61	J/mol×K	929.64	Joback Method
cpg	1070.38	J/mol×K	968.77	Joback Method
cpg	1100.77	J/mol×K	1007.89	Joback Method
cpg	1133.19	J/mol×K	1047.02	Joback Method
cpg	1168.10	J/mol×K	1086.14	Joback Method
cpg	1205.91	J/mol×K	1125.27	Joback Method
cpg	1247.07	J/mol×K	1164.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392959&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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