[14C1]GA25 methyl ester

Inchi: InChI=1S/C23H32O6/c1-13-11-22-12-14(13)7-8-15(22)23(20(26)29-5)10-6-9-21(2,19(25)
InchiKey: CVVOOYMCPNGYQG-VBYMKQBWSA-N
Formula: C23H32O6
SMILES: C=C1CC23CC1CCC2C1(C(=O)OC)CCCC(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 404.50

Physical Properties

Property code	Value	Unit	Source
gf	-338.80	kJ/mol	Joback Method
hf	-910.79	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	90.21	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.291		Crippen Method
mcvol	309.510	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	980.15	K	Joback Method
tc	1216.30	K	Joback Method
tf	699.31	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.01	J/mol×K	980.15	Joback Method
cpg	1178.78	J/mol×K	1019.51	Joback Method
cpg	1212.49	J/mol×K	1058.87	Joback Method
cpg	1248.56	J/mol×K	1098.23	Joback Method
cpg	1287.41	J/mol×K	1137.58	Joback Method
cpg	1329.47	J/mol×K	1176.94	Joback Method
cpg	1375.16	J/mol×K	1216.30	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=R392919&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