[14C] 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-YDEQTJGSSA-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	2429.00		NIST Webbook
rinpol	2429.00		NIST Webbook
rinpol	2428.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2428.00		NIST Webbook
rinpol	2455.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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