[14C1]GA9 methyl ester

Inchi: InChI=1S/C20H26O4/c1-11-9-19-10-12(11)5-6-13(19)20-8-4-7-18(2,17(22)24-20)15(20)1
InchiKey: GKRMJALKMNRHGF-HAYZNOEYSA-N
Formula: C20H26O4
SMILES: C=C1CC23CC1CCC2C12CCCC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-24.37	kJ/mol	Joback Method
hf	-529.67	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.254		Crippen Method
mcvol	248.940	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	2299.00		NIST Webbook
tb	860.84	K	Joback Method
tc	1110.66	K	Joback Method
tf	641.67	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.72	J/mol×K	860.84	Joback Method
cpg	912.88	J/mol×K	902.48	Joback Method
cpg	941.45	J/mol×K	944.11	Joback Method
cpg	971.97	J/mol×K	985.75	Joback Method
cpg	1005.00	J/mol×K	1027.39	Joback Method
cpg	1041.11	J/mol×K	1069.03	Joback Method
cpg	1080.84	J/mol×K	1110.66	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=R392939&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