2,3-Dehydro-[14C]GA9 methyl ester

Other names: 2,3-Dehydro-GA9 methyl ester
Inchi: InChI=1S/C20H24O4/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: VWPPKHJWYLVPJJ-RKWHRFJJSA-N
Formula: C20H24O4
SMILES: C=C1CC23CC1CCC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
gf	5.59	kJ/mol	Joback Method
hf	-471.89	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.030		Crippen Method
mcvol	244.640	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	860.00	K	Joback Method
tc	1111.71	K	Joback Method
tf	642.43	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.88	J/mol×K	860.00	Joback Method
cpg	883.23	J/mol×K	901.95	Joback Method
cpg	911.08	J/mol×K	943.90	Joback Method
cpg	941.00	J/mol×K	985.85	Joback Method
cpg	973.57	J/mol×K	1027.81	Joback Method
cpg	1009.34	J/mol×K	1069.76	Joback Method

cpg	1048.91	J/mol×K	1111.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190951&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