[14C4]GA15 methyl ester TMS ether

Inchi: InChI=1S/C21H28O4/c1-12-9-21-10-13(12)5-6-14(21)20-8-4-7-19(2,18(23)25-11-20)16(2
InchiKey: SDNANUVFTHNCBP-XDCUROHDSA-N
Formula: C21H28O4
SMILES: C=C1CC23CC1CCC2C12CCCC(C)(C(=O)OC1)C2C3C(=O)OC
Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-28.05	kJ/mol	Joback Method
hf	-556.47	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.501		Crippen Method
mcvol	263.030	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	887.99	K	Joback Method
tc	1139.83	K	Joback Method
tf	649.42	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.19	J/mol×K	887.99	Joback Method
cpg	983.54	J/mol×K	929.96	Joback Method
cpg	1014.48	J/mol×K	971.94	Joback Method
cpg	1047.57	J/mol×K	1013.91	Joback Method
cpg	1083.38	J/mol×K	1055.88	Joback Method
cpg	1122.47	J/mol×K	1097.86	Joback Method
cpg	1165.40	J/mol×K	1139.83	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=R392944&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