16«alpha»,17-dihydroxy-16,17-dihydroGA4-17-O-«
permethylated

Inchi: InChI=1S/C32H50O12/c1-29-20(36-3)11-12-32(44-28(29)34)19-10-9-17-13-30(19,21(25(
InchiKey: DYZOPYIERZRHQX-QULGNCHQSA-N
Formula: C32H50O12
SMILES: COCC1OC(OCC2(OC)CC34CC2CCC3C23CCC(OC)C(C)(C(=O)O2)C3C4C(=O)OC)C(C
Mol. weight [g/mol]: 626.73

Physical Properties

Property code	Value	Unit	Source
gf	-824.83	kJ/mol	Joback Method
hf	-1971.61	kJ/mol	Joback Method
hfus	66.89	kJ/mol	Joback Method
hvap	119.38	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.141		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
pc	804.79	kPa	Joback Method
rinpol	3775.00		NIST Webbook
rinpol	3780.00		NIST Webbook
rinpol	3775.00		NIST Webbook
tb	1311.90	K	Joback Method
tc	1621.26	K	Joback Method
tf	951.25	K	Joback Method
vc	1.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2234.19	J/mol×K	1311.90	Joback Method
cpg	2324.27	J/mol×K	1363.46	Joback Method
cpg	2422.92	J/mol×K	1415.02	Joback Method
cpg	2531.13	J/mol×K	1466.58	Joback Method
cpg	2649.89	J/mol×K	1518.14	Joback Method
cpg	2780.19	J/mol×K	1569.70	Joback Method
cpg	2923.02	J/mol×K	1621.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R259882&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