22R-epi-17«beta»(H),21«beta»(H)-Hopanoic acid methyl ester

Inchi: InChI=1S/C31H52O2/c1-20(26(32)33-8)21-12-17-28(4)22(21)13-18-30(6)24(28)10-11-25

InchiKey: YUHMMAGHEGZDPT-VKVPZFAZSA-N

Formula: C31H52O2

SMILES: COC(=O)C(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C

Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	138.93	kJ/mol	Joback Method
hf	-631.71	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.287		Crippen Method
mcvol	400.790	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	3554.00		NIST Webbook
rinpol	3554.00		NIST Webbook
tb	1021.70	K	Joback Method
tc	1268.46	K	Joback Method
tf	663.17	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1634.26	J/mol×K	1021.70	Joback Method
cpg	1691.17	J/mol×K	1062.83	Joback Method
cpg	1753.16	J/mol×K	1103.95	Joback Method
cpg	1821.06	J/mol×K	1145.08	Joback Method
cpg	1895.67	J/mol×K	1186.21	Joback Method
cpg	1977.82	J/mol×K	1227.33	Joback Method
cpg	2068.33	J/mol×K	1268.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419044&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

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