17«beta»(H),21«beta»(H)-Homohopanoic acid methyl ester

Inchi: InChI=1S/C32H54O2/c1-21(20-27(33)34-8)22-12-17-29(4)23(22)13-18-31(6)25(29)10-11

InchiKey: BTHZNHKNYAGYBB-OVNILPMUSA-N

Formula: C32H54O2

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

Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	147.35	kJ/mol	Joback Method
hf	-652.35	kJ/mol	Joback Method
hfus	29.84	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	8.677		Crippen Method
mcvol	414.880	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	3714.00		NIST Webbook
tb	1044.58	K	Joback Method
tc	1290.99	K	Joback Method
tf	674.44	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1717.88	J/mol×K	1044.58	Joback Method
cpg	1778.23	J/mol×K	1085.65	Joback Method
cpg	1844.05	J/mol×K	1126.72	Joback Method
cpg	1916.16	J/mol×K	1167.78	Joback Method
cpg	1995.38	J/mol×K	1208.85	Joback Method
cpg	2082.52	J/mol×K	1249.92	Joback Method
cpg	2178.41	J/mol×K	1290.99	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=R419024&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