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

Inchi: InChI=1S/C33H56O2/c1-22(10-13-28(34)35-8)23-14-19-30(4)24(23)15-20-32(6)26(30)11

InchiKey: ORWUNXLWVUEFHW-ZAYZLFOQSA-N

Formula: C33H56O2

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

Mol. weight [g/mol]: 484.80

Physical Properties

Property code	Value	Unit	Source
gf	155.77	kJ/mol	Joback Method
hf	-672.99	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	9.067		Crippen Method
mcvol	428.970	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	3722.00		NIST Webbook
tb	1067.46	K	Joback Method
tc	1314.47	K	Joback Method
tf	685.71	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1803.86	J/mol×K	1067.46	Joback Method
cpg	1868.10	J/mol×K	1108.63	Joback Method
cpg	1938.24	J/mol×K	1149.80	Joback Method
cpg	2015.12	J/mol×K	1190.96	Joback Method
cpg	2099.56	J/mol×K	1232.13	Joback Method
cpg	2192.41	J/mol×K	1273.30	Joback Method
cpg	2294.48	J/mol×K	1314.47	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=R419004&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

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