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

Inchi: InChI=1S/C34H58O2/c1-23(11-9-12-29(35)36-8)24-15-20-31(4)25(24)16-21-33(6)27(31)
InchiKey: UAKBHIYWVXYFFB-GXVGMDOOSA-N
Formula: C34H58O2
SMILES: COC(=O)CCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 498.82

Physical Properties

Property code	Value	Unit	Source
gf	164.19	kJ/mol	Joback Method
hf	-693.63	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	9.457		Crippen Method
mcvol	443.060	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3941.00		NIST Webbook
tb	1090.34	K	Joback Method
tc	1338.95	K	Joback Method
tf	696.98	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1892.31	J/mol×K	1090.34	Joback Method
cpg	1960.93	J/mol×K	1131.77	Joback Method
cpg	2035.97	J/mol×K	1173.21	Joback Method
cpg	2118.26	J/mol×K	1214.64	Joback Method
cpg	2208.67	J/mol×K	1256.08	Joback Method
cpg	2308.04	J/mol×K	1297.51	Joback Method
cpg	2417.22	J/mol×K	1338.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419039&Units=SI

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