28-Norhomohopan-31-oic acid methyl ester

Inchi: InChI=1S/C31H52O2/c1-20(19-27(32)33-7)21-9-10-23-22(21)13-17-30(5)24(23)11-12-26
InchiKey: AYLCQMKAZURMNK-GLUWJVINSA-N
Formula: C31H52O2
SMILES: COC(=O)CC(C)C1CCC2C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	144.42	kJ/mol	Joback Method
hf	-646.95	kJ/mol	Joback Method
hfus	33.55	kJ/mol	Joback Method
hvap	87.82	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.287		Crippen Method
mcvol	400.790	ml/mol	McGowan Method
pc	904.52	kPa	Joback Method
rinpol	3541.00		NIST Webbook
tb	1021.46	K	Joback Method
tc	1264.14	K	Joback Method
tf	639.27	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1623.86	J/mol×K	1021.46	Joback Method
cpg	1673.59	J/mol×K	1061.91	Joback Method
cpg	1726.86	J/mol×K	1102.35	Joback Method
cpg	1784.32	J/mol×K	1142.80	Joback Method
cpg	1846.64	J/mol×K	1183.25	Joback Method
cpg	1914.47	J/mol×K	1223.69	Joback Method
cpg	1988.48	J/mol×K	1264.14	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=R419099&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