22S-epi-28-Norhopanoic acid methyl ester

Inchi: InChI=1S/C30H50O2/c1-19(26(31)32-7)20-9-10-22-21(20)13-17-29(5)23(22)11-12-25-28
InchiKey: XPHZXWVRRHPDNR-QDDBVERGSA-N
Formula: C30H50O2
SMILES: COC(=O)C(C)C1CCC2C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 442.72

Physical Properties

Property code	Value	Unit	Source
gf	136.00	kJ/mol	Joback Method
hf	-626.31	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	85.59	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.897		Crippen Method
mcvol	386.700	ml/mol	McGowan Method
pc	959.10	kPa	Joback Method
rinpol	3409.00		NIST Webbook
tb	998.58	K	Joback Method
tc	1241.82	K	Joback Method
tf	628.00	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1545.48	J/mol×K	998.58	Joback Method
cpg	1592.76	J/mol×K	1039.12	Joback Method
cpg	1643.27	J/mol×K	1079.66	Joback Method
cpg	1697.68	J/mol×K	1120.20	Joback Method
cpg	1756.64	J/mol×K	1160.74	Joback Method
cpg	1820.82	J/mol×K	1201.28	Joback Method
cpg	1890.87	J/mol×K	1241.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419079&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