28-bishomopan-32-oic acid methyl ester

Inchi: InChI=1S/C32H54O2/c1-21(9-14-28(33)34-7)22-10-11-24-23(22)15-19-31(5)25(24)12-13
InchiKey: NUZFPUBWBRFCKH-UYSGOOEHSA-N
Formula: C32H54O2
SMILES: COC(=O)CCC(C)C1CCC2C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	152.84	kJ/mol	Joback Method
hf	-667.59	kJ/mol	Joback Method
hfus	36.14	kJ/mol	Joback Method
hvap	90.04	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	8.677		Crippen Method
mcvol	414.880	ml/mol	McGowan Method
pc	854.46	kPa	Joback Method
rinpol	3657.00		NIST Webbook
tb	1044.34	K	Joback Method
tc	1287.38	K	Joback Method
tf	650.54	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1704.12	J/mol×K	1044.34	Joback Method
cpg	1756.65	J/mol×K	1084.85	Joback Method
cpg	1813.04	J/mol×K	1125.35	Joback Method
cpg	1873.98	J/mol×K	1165.86	Joback Method
cpg	1940.12	J/mol×K	1206.37	Joback Method
cpg	2012.13	J/mol×K	1246.88	Joback Method
cpg	2090.68	J/mol×K	1287.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419084&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