Methyl olean-3-oxo-28-oate

Inchi: InChI=1S/C31H50O3/c1-26(2)15-17-31(25(33)34-8)18-16-29(6)20(21(31)19-26)9-10-23-
InchiKey: WZVIOBOAONWCSW-UHFFFAOYSA-N
Formula: C31H50O3
SMILES: COC(=O)C12CCC(C)(C)CC1C1CCC3C4(C)CCC(=O)C(C)(C)C4CCC3(C)C1(C)CC2
Mol. weight [g/mol]: 470.73

Physical Properties

Property code	Value	Unit	Source
gf	1.19	kJ/mol	Joback Method
hf	-755.05	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.610		Crippen Method
mcvol	402.360	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	3560.00		NIST Webbook
tb	1094.47	K	Joback Method
tc	1357.40	K	Joback Method
tf	766.77	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1757.39	J/mol×K	1094.47	Joback Method
cpg	1835.28	J/mol×K	1138.29	Joback Method
cpg	1921.76	J/mol×K	1182.11	Joback Method
cpg	2017.91	J/mol×K	1225.93	Joback Method
cpg	2124.79	J/mol×K	1269.76	Joback Method
cpg	2243.48	J/mol×K	1313.58	Joback Method
cpg	2375.04	J/mol×K	1357.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R558802&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